



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 08:13 PM EDT

PDB ID : 2N4P  
BMRB ID : 25675  
Title : Solution structure of the n-terminal domain of tdp-43  
Authors : Mompean, M.; Romano, V.; Pantoja-Uceda, D.; Stuani, C.; Baralle, F.; Burratti, E.; Laurents, D.V.  
Deposited on : 2015-06-26

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.33

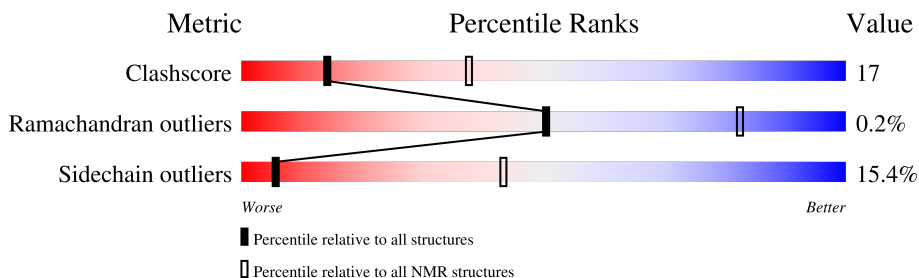
# 1 Overall quality at a glance

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 (#Entries) | NMR archive (#Entries) |
|-----------------------|--------------------------|------------------------|
| Clashscore            | 158937                   | 12864                  |
| Ramachandran outliers | 154571                   | 11451                  |
| Sidechain outliers    | 154315                   | 11428                  |

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     | 89     |                  |

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 11 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:16-A:57, A:65-A:89 (67) | 0.26              | 11           |

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 2 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1344 atoms, of which 653 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TAR DNA-binding protein 43.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
|     |       |          | Total | C   | H   | N   | O   | S |       |
| 1   | A     | 89       | 1344  | 427 | 653 | 125 | 134 | 5 | 0     |

There are 12 discrepancies between the modelled and reference sequences:

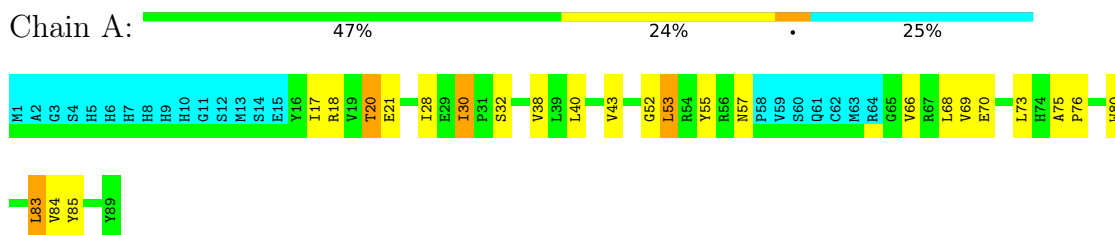
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | MET      | -      | expression tag | UNP Q13148 |
| A     | 2       | ALA      | -      | expression tag | UNP Q13148 |
| A     | 3       | GLY      | -      | expression tag | UNP Q13148 |
| A     | 4       | SER      | -      | expression tag | UNP Q13148 |
| A     | 5       | HIS      | -      | expression tag | UNP Q13148 |
| A     | 6       | HIS      | -      | expression tag | UNP Q13148 |
| A     | 7       | HIS      | -      | expression tag | UNP Q13148 |
| A     | 8       | HIS      | -      | expression tag | UNP Q13148 |
| A     | 9       | HIS      | -      | expression tag | UNP Q13148 |
| A     | 10      | HIS      | -      | expression tag | UNP Q13148 |
| A     | 11      | GLY      | -      | expression tag | UNP Q13148 |
| A     | 12      | SER      | -      | expression tag | UNP Q13148 |

## 4 Residue-property plots

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

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

- Molecule 1: TAR DNA-binding protein 43

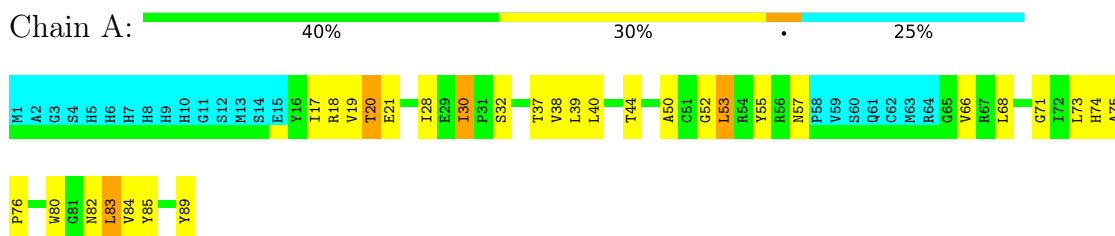


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

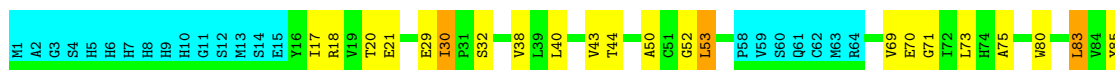
- Molecule 1: TAR DNA-binding protein 43



#### 4.2.2 Score per residue for model 2

- Molecule 1: TAR DNA-binding protein 43





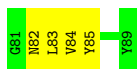
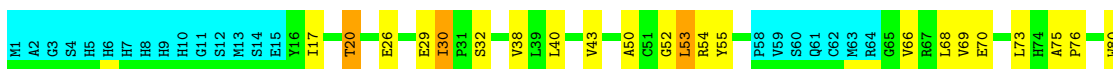
### 4.2.3 Score per residue for model 3

- Molecule 1: TAR DNA-binding protein 43



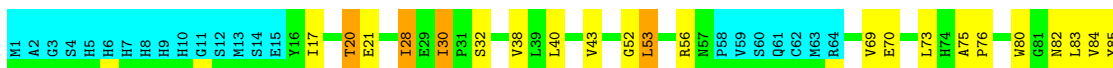
### 4.2.4 Score per residue for model 4

- Molecule 1: TAR DNA-binding protein 43



### 4.2.5 Score per residue for model 5

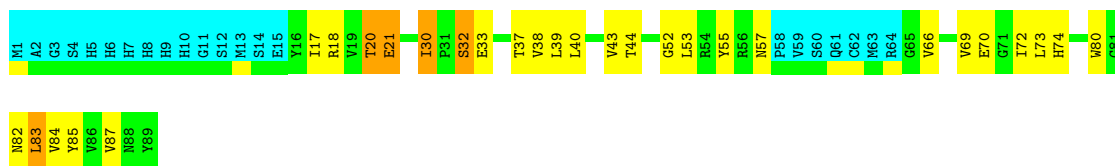
- Molecule 1: TAR DNA-binding protein 43



### 4.2.6 Score per residue for model 6

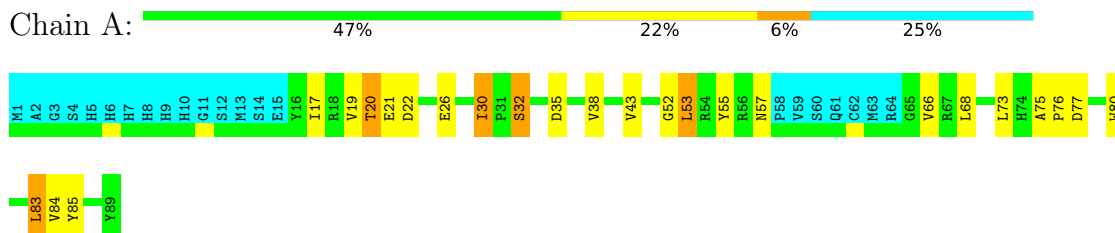
- Molecule 1: TAR DNA-binding protein 43





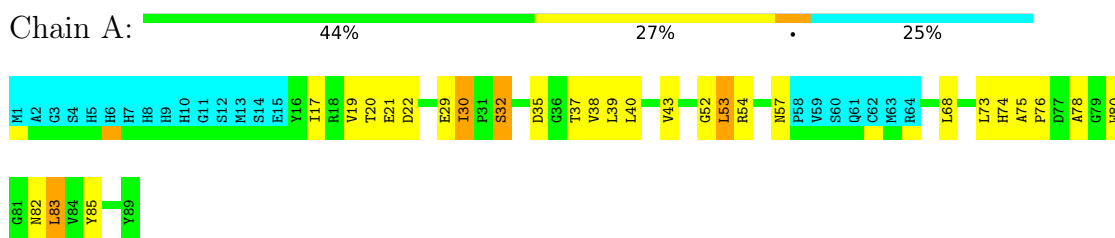
#### 4.2.7 Score per residue for model 7

- Molecule 1: TAR DNA-binding protein 43



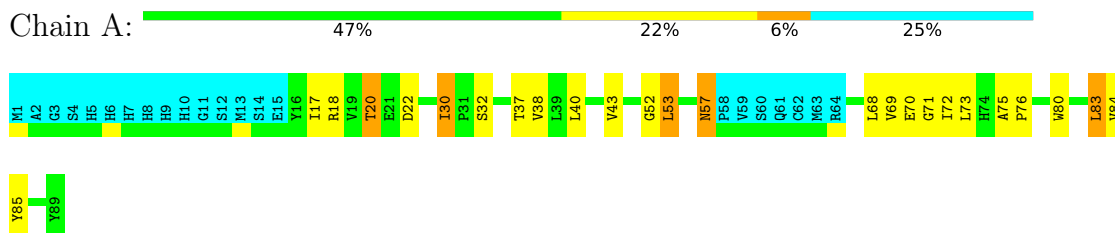
#### 4.2.8 Score per residue for model 8

- Molecule 1: TAR DNA-binding protein 43



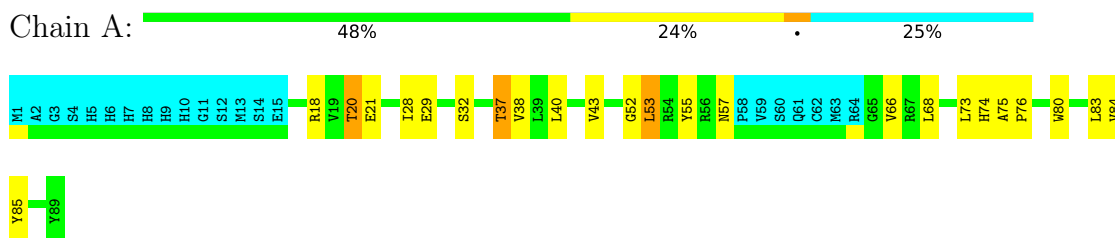
#### 4.2.9 Score per residue for model 9

- Molecule 1: TAR DNA-binding protein 43



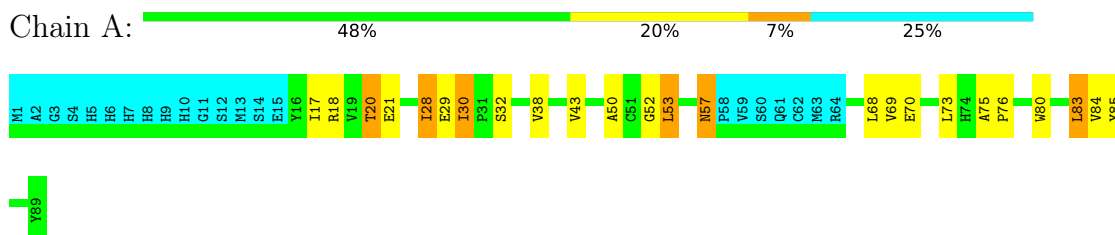
#### 4.2.10 Score per residue for model 10

- Molecule 1: TAR DNA-binding protein 43



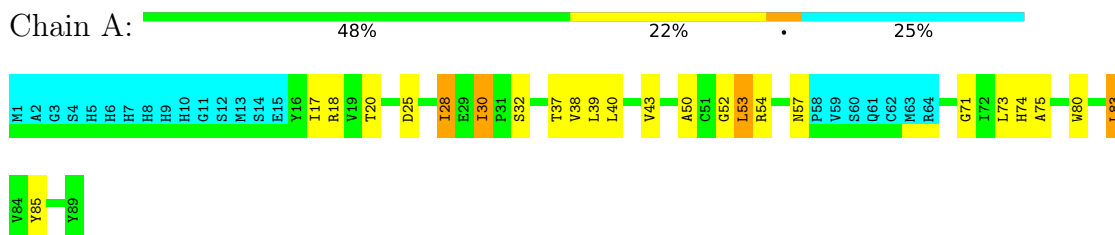
#### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: TAR DNA-binding protein 43



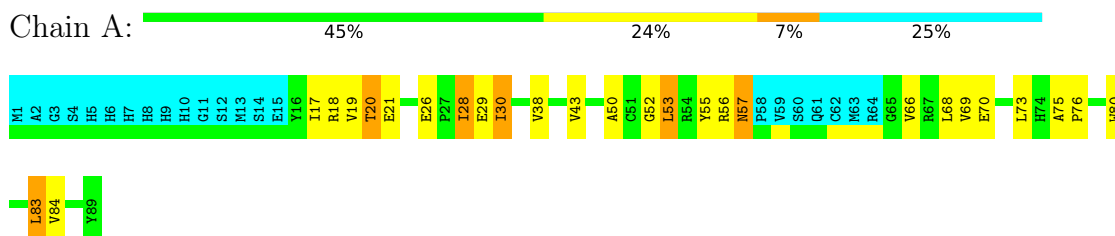
#### 4.2.12 Score per residue for model 12

- Molecule 1: TAR DNA-binding protein 43



#### 4.2.13 Score per residue for model 13

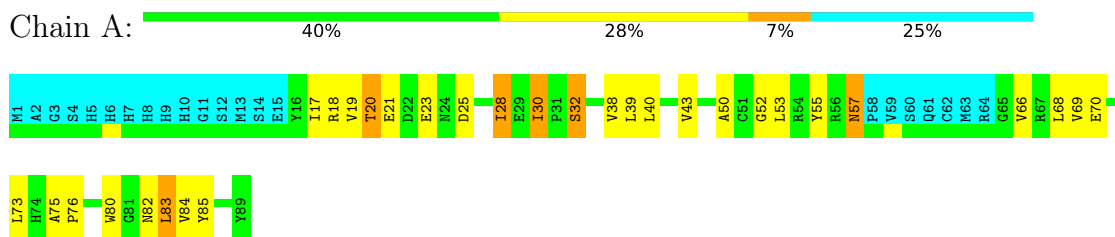
- Molecule 1: TAR DNA-binding protein 43





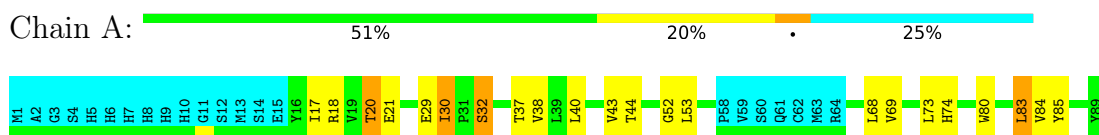
#### 4.2.14 Score per residue for model 14

- Molecule 1: TAR DNA-binding protein 43



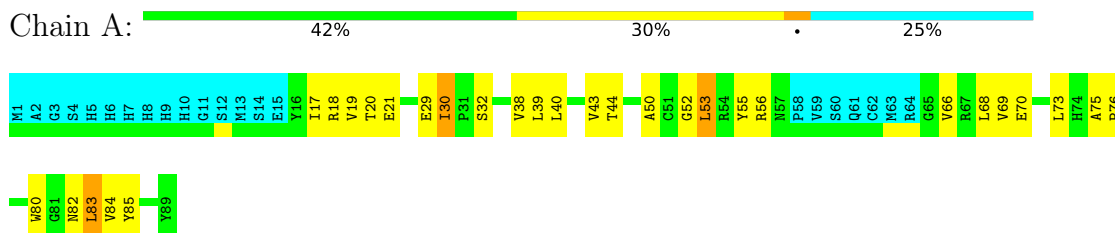
#### 4.2.15 Score per residue for model 15

- Molecule 1: TAR DNA-binding protein 43



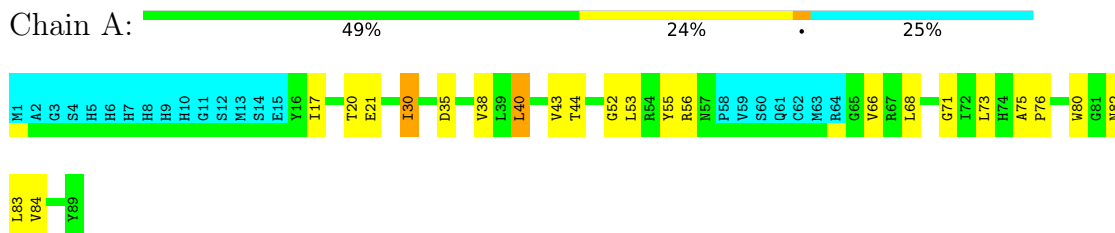
#### 4.2.16 Score per residue for model 16

- Molecule 1: TAR DNA-binding protein 43



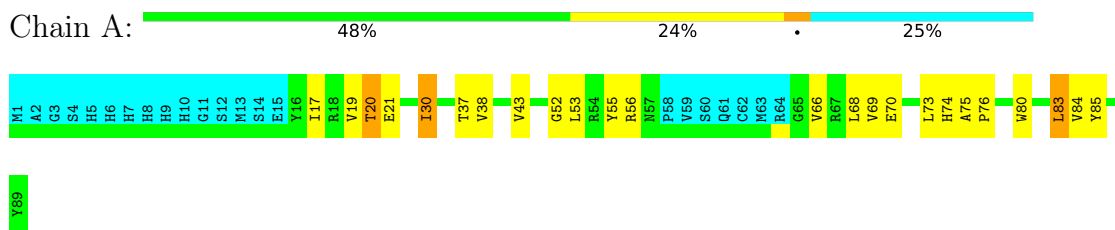
#### 4.2.17 Score per residue for model 17

- Molecule 1: TAR DNA-binding protein 43



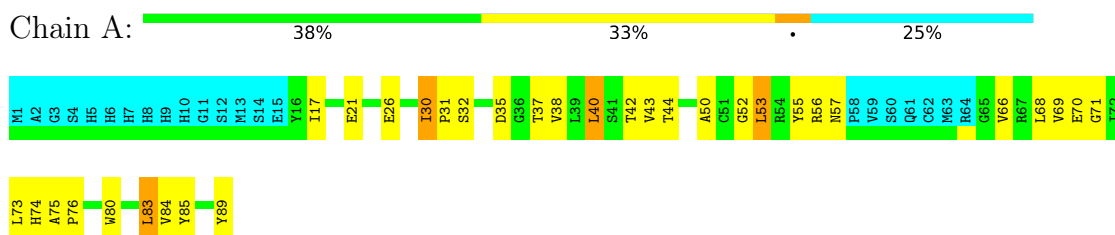
#### 4.2.18 Score per residue for model 18

- Molecule 1: TAR DNA-binding protein 43



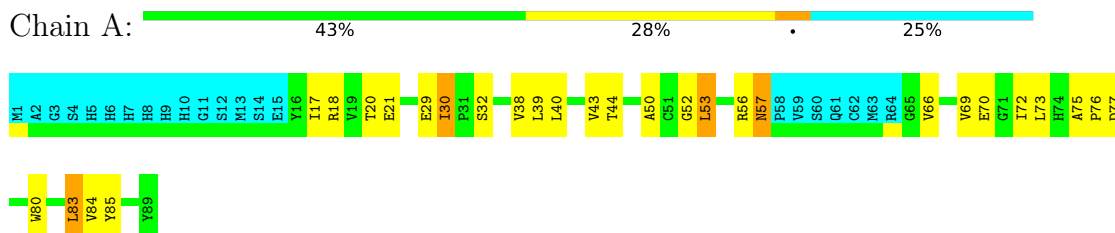
#### 4.2.19 Score per residue for model 19

- Molecule 1: TAR DNA-binding protein 43



#### 4.2.20 Score per residue for model 20

- Molecule 1: TAR DNA-binding protein 43



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *ENERGY MINIMIZATION*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

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

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

| Chemical shift file(s)                       | working_cs.cif |
|--|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1013           |
| Number of shifts mapped to atoms             | 1013           |
| 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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 521   | 497      | 496      | 18±3    |
| All | All   | 10420 | 9940     | 9920     | 354     |

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 17.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:20:THR:HG23 | 1:A:84:VAL:HG12 | 0.92     | 1.42        | 13     | 1     |
| 1:A:43:VAL:HG21 | 1:A:73:LEU:HD23 | 0.81     | 1.51        | 8      | 19    |
| 1:A:28:ILE:HD11 | 1:A:30:ILE:HG23 | 0.71     | 1.61        | 12     | 5     |
| 1:A:53:LEU:HD12 | 1:A:85:TYR:CE1  | 0.67     | 2.24        | 9      | 5     |
| 1:A:40:LEU:HD12 | 1:A:71:GLY:CA   | 0.65     | 2.22        | 1      | 6     |
| 1:A:40:LEU:HD12 | 1:A:71:GLY:HA3  | 0.61     | 1.71        | 17     | 5     |
| 1:A:52:GLY:C    | 1:A:53:LEU:HD12 | 0.60     | 2.17        | 17     | 1     |
| 1:A:43:VAL:HG21 | 1:A:73:LEU:CD2  | 0.60     | 2.26        | 7      | 6     |
| 1:A:20:THR:CG2  | 1:A:84:VAL:HG22 | 0.60     | 2.26        | 4      | 11    |
| 1:A:53:LEU:HD12 | 1:A:85:TYR:CE2  | 0.60     | 2.31        | 3      | 9     |
| 1:A:40:LEU:O    | 1:A:40:LEU:HD13 | 0.59     | 1.96        | 4      | 6     |
| 1:A:53:LEU:HD13 | 1:A:85:TYR:CD2  | 0.59     | 2.33        | 14     | 4     |
| 1:A:40:LEU:HD13 | 1:A:40:LEU:O    | 0.58     | 1.98        | 14     | 1     |
| 1:A:55:TYR:CZ   | 1:A:66:VAL:HG22 | 0.58     | 2.34        | 4      | 11    |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:53:LEU:HD22 | 1:A:85:TYR:CE2  | 0.58     | 2.33        | 18     | 4     |
| 1:A:52:GLY:C    | 1:A:53:LEU:HD13 | 0.58     | 2.19        | 9      | 15    |
| 1:A:53:LEU:HD22 | 1:A:85:TYR:CD2  | 0.57     | 2.34        | 15     | 4     |
| 1:A:28:ILE:CD1  | 1:A:30:ILE:HG23 | 0.57     | 2.30        | 11     | 4     |
| 1:A:17:ILE:HG23 | 1:A:30:ILE:HG13 | 0.56     | 1.77        | 7      | 19    |
| 1:A:20:THR:HG23 | 1:A:84:VAL:HG22 | 0.56     | 1.77        | 4      | 11    |
| 1:A:83:LEU:HD13 | 1:A:83:LEU:N    | 0.56     | 2.16        | 8      | 7     |
| 1:A:52:GLY:O    | 1:A:53:LEU:HD23 | 0.56     | 2.01        | 15     | 4     |
| 1:A:19:VAL:HG12 | 1:A:83:LEU:HD12 | 0.55     | 1.77        | 7      | 4     |
| 1:A:38:VAL:HG23 | 1:A:80:TRP:CZ2  | 0.55     | 2.36        | 8      | 20    |
| 1:A:56:ARG:HB3  | 1:A:84:VAL:HG13 | 0.55     | 1.78        | 19     | 4     |
| 1:A:20:THR:HG23 | 1:A:84:VAL:HG13 | 0.55     | 1.77        | 18     | 1     |
| 1:A:55:TYR:CD1  | 1:A:83:LEU:HD11 | 0.54     | 2.37        | 6      | 3     |
| 1:A:66:VAL:HG12 | 1:A:73:LEU:HD12 | 0.54     | 1.80        | 20     | 1     |
| 1:A:75:ALA:HB2  | 1:A:80:TRP:CE2  | 0.53     | 2.39        | 3      | 14    |
| 1:A:40:LEU:O    | 1:A:44:THR:HG23 | 0.53     | 2.04        | 15     | 7     |
| 1:A:37:THR:HG22 | 1:A:74:HIS:CG   | 0.53     | 2.38        | 18     | 2     |
| 1:A:83:LEU:H    | 1:A:83:LEU:HD13 | 0.52     | 1.62        | 19     | 2     |
| 1:A:83:LEU:HD13 | 1:A:83:LEU:H    | 0.52     | 1.63        | 20     | 7     |
| 1:A:69:VAL:HG22 | 1:A:70:GLU:HG3  | 0.52     | 1.80        | 19     | 5     |
| 1:A:50:ALA:HB1  | 1:A:53:LEU:HD11 | 0.52     | 1.82        | 1      | 9     |
| 1:A:53:LEU:HD23 | 1:A:73:LEU:HG   | 0.51     | 1.83        | 1      | 5     |
| 1:A:70:GLU:CD   | 1:A:72:ILE:HD12 | 0.50     | 2.26        | 20     | 1     |
| 1:A:19:VAL:HG12 | 1:A:83:LEU:CD2  | 0.49     | 2.37        | 8      | 2     |
| 1:A:40:LEU:HD12 | 1:A:71:GLY:HA2  | 0.49     | 1.84        | 1      | 2     |
| 1:A:40:LEU:HD23 | 1:A:40:LEU:O    | 0.49     | 2.08        | 1      | 3     |
| 1:A:56:ARG:HB3  | 1:A:84:VAL:HG23 | 0.49     | 1.83        | 13     | 1     |
| 1:A:31:PRO:O    | 1:A:42:THR:HG21 | 0.49     | 2.07        | 19     | 1     |
| 1:A:66:VAL:CG1  | 1:A:73:LEU:HD12 | 0.48     | 2.38        | 20     | 1     |
| 1:A:69:VAL:HG22 | 1:A:70:GLU:HG2  | 0.47     | 1.85        | 2      | 5     |
| 1:A:82:ASN:C    | 1:A:83:LEU:HD13 | 0.47     | 2.29        | 8      | 1     |
| 1:A:52:GLY:C    | 1:A:53:LEU:HD23 | 0.47     | 2.30        | 15     | 4     |
| 1:A:37:THR:HG22 | 1:A:74:HIS:HA   | 0.47     | 1.87        | 8      | 6     |
| 1:A:53:LEU:HD12 | 1:A:85:TYR:CD2  | 0.46     | 2.45        | 1      | 2     |
| 1:A:32:SER:CB   | 1:A:38:VAL:HG22 | 0.46     | 2.40        | 3      | 4     |
| 1:A:52:GLY:O    | 1:A:53:LEU:HD13 | 0.46     | 2.11        | 9      | 1     |
| 1:A:53:LEU:HD22 | 1:A:53:LEU:N    | 0.46     | 2.26        | 9      | 1     |
| 1:A:57:ASN:OD1  | 1:A:83:LEU:HD12 | 0.46     | 2.11        | 20     | 3     |
| 1:A:32:SER:HB2  | 1:A:38:VAL:HG22 | 0.45     | 1.87        | 6      | 12    |
| 1:A:83:LEU:CD2  | 1:A:83:LEU:C    | 0.45     | 2.85        | 16     | 8     |
| 1:A:39:LEU:HD23 | 1:A:72:ILE:HG12 | 0.45     | 1.88        | 20     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:33:GLU:HG2  | 1:A:39:LEU:HD23 | 0.45     | 1.89        | 6      | 1     |
| 1:A:50:ALA:HB1  | 1:A:53:LEU:HD21 | 0.45     | 1.88        | 14     | 1     |
| 1:A:19:VAL:HG12 | 1:A:83:LEU:CD1  | 0.44     | 2.42        | 7      | 1     |
| 1:A:32:SER:HB3  | 1:A:38:VAL:HG22 | 0.44     | 1.88        | 4      | 3     |
| 1:A:75:ALA:HB1  | 1:A:76:PRO:HD2  | 0.44     | 1.90        | 8      | 16    |
| 1:A:83:LEU:C    | 1:A:83:LEU:CD2  | 0.44     | 2.86        | 20     | 1     |
| 1:A:68:LEU:HD13 | 1:A:68:LEU:C    | 0.44     | 2.33        | 7      | 11    |
| 1:A:68:LEU:O    | 1:A:68:LEU:HD13 | 0.44     | 2.13        | 18     | 1     |
| 1:A:68:LEU:C    | 1:A:68:LEU:HD13 | 0.43     | 2.33        | 19     | 2     |
| 1:A:69:VAL:O    | 1:A:70:GLU:CG   | 0.43     | 2.66        | 18     | 2     |
| 1:A:40:LEU:O    | 1:A:40:LEU:HD23 | 0.43     | 2.13        | 2      | 1     |
| 1:A:19:VAL:HG12 | 1:A:83:LEU:HD23 | 0.42     | 1.91        | 18     | 1     |
| 1:A:40:LEU:HD23 | 1:A:44:THR:HG23 | 0.42     | 1.89        | 1      | 1     |
| 1:A:68:LEU:HD22 | 1:A:69:VAL:N    | 0.42     | 2.29        | 18     | 3     |
| 1:A:37:THR:HB   | 1:A:72:ILE:HG22 | 0.42     | 1.91        | 9      | 2     |
| 1:A:17:ILE:HD12 | 1:A:80:TRP:CE3  | 0.42     | 2.50        | 7      | 1     |
| 1:A:53:LEU:N    | 1:A:53:LEU:HD22 | 0.41     | 2.30        | 2      | 1     |
| 1:A:19:VAL:O    | 1:A:28:ILE:HG22 | 0.41     | 2.15        | 13     | 2     |
| 1:A:21:GLU:HG2  | 1:A:87:VAL:HG13 | 0.41     | 1.93        | 6      | 1     |
| 1:A:20:THR:O    | 1:A:84:VAL:HG13 | 0.41     | 2.16        | 6      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 66/89 (74%)     | 64±2 (97±2%) | 2±1 (3±2%) | 0±0 (0±0%) | 50          | 82 |
| All | All   | 1320/1780 (74%) | 1278 (97%)   | 40 (3%)    | 2 (0%)     | 50          | 82 |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 78  | ALA  | 1              |
| 1   | A     | 37  | THR  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers    | Percentiles |
|-----|-------|-----------------|--------------|-------------|-------------|
| 1   | A     | 56/75 (75%)     | 47±2 (85±4%) | 9±2 (15±4%) | <b>6</b> 43 |
| All | All   | 1120/1500 (75%) | 948 (85%)    | 172 (15%)   | <b>6</b> 43 |

All 22 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     | 20  | THR  | 19             |
| 1   | A     | 30  | ILE  | 19             |
| 1   | A     | 83  | LEU  | 19             |
| 1   | A     | 21  | GLU  | 17             |
| 1   | A     | 53  | LEU  | 15             |
| 1   | A     | 18  | ARG  | 12             |
| 1   | A     | 57  | ASN  | 12             |
| 1   | A     | 29  | GLU  | 9              |
| 1   | A     | 82  | ASN  | 7              |
| 1   | A     | 28  | ILE  | 6              |
| 1   | A     | 32  | SER  | 6              |
| 1   | A     | 39  | LEU  | 5              |
| 1   | A     | 26  | GLU  | 4              |
| 1   | A     | 35  | ASP  | 4              |
| 1   | A     | 54  | ARG  | 3              |
| 1   | A     | 22  | ASP  | 3              |
| 1   | A     | 40  | LEU  | 3              |
| 1   | A     | 89  | TYR  | 2              |
| 1   | A     | 56  | ARG  | 2              |
| 1   | A     | 77  | ASP  | 2              |
| 1   | A     | 25  | ASP  | 2              |
| 1   | A     | 23  | GLU  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.



## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 87% 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 [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                  | 1013 |
| Number of shifts mapped to atoms        | 1013 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 4    |

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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action        |
|------------------------|----------|---------------------------------|-------------------------|
| $^{13}\text{C}_\alpha$ | 84       | $0.16 \pm 0.11$                 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$  | 77       | $0.27 \pm 0.17$                 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$       | 81       | $0.15 \pm 0.16$                 | None needed (< 0.5 ppm) |
| $^{15}\text{N}$        | 81       | $0.37 \pm 0.52$                 | None needed (< 0.5 ppm) |

#### 7.1.3 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 90%, i.e. 803 atoms were assigned a chemical shift out of a possible 888. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 326/334 (98%) | 137/137 (100%) | 126/134 (94%)   | 63/63 (100%)    |
| Sidechain | 431/488 (88%) | 292/318 (92%)  | 130/153 (85%)   | 9/17 (53%)      |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 46/66 (70%)   | 28/31 (90%)    | 17/32 (53%)     | 1/3 (33%)       |
| Overall  | 803/888 (90%) | 457/486 (94%)  | 273/319 (86%)   | 73/83 (88%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1013 atoms were assigned a chemical shift out of a possible 1167. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 423/444 (95%)   | 177/182 (97%)  | 165/178 (93%)   | 81/84 (96%)     |
| Sidechain | 520/609 (85%)   | 352/398 (88%)  | 157/190 (83%)   | 11/21 (52%)     |
| Aromatic  | 70/114 (61%)    | 40/55 (73%)    | 29/44 (66%)     | 1/15 (7%)       |
| Overall   | 1013/1167 (87%) | 569/635 (90%)  | 351/412 (85%)   | 93/120 (78%)    |

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

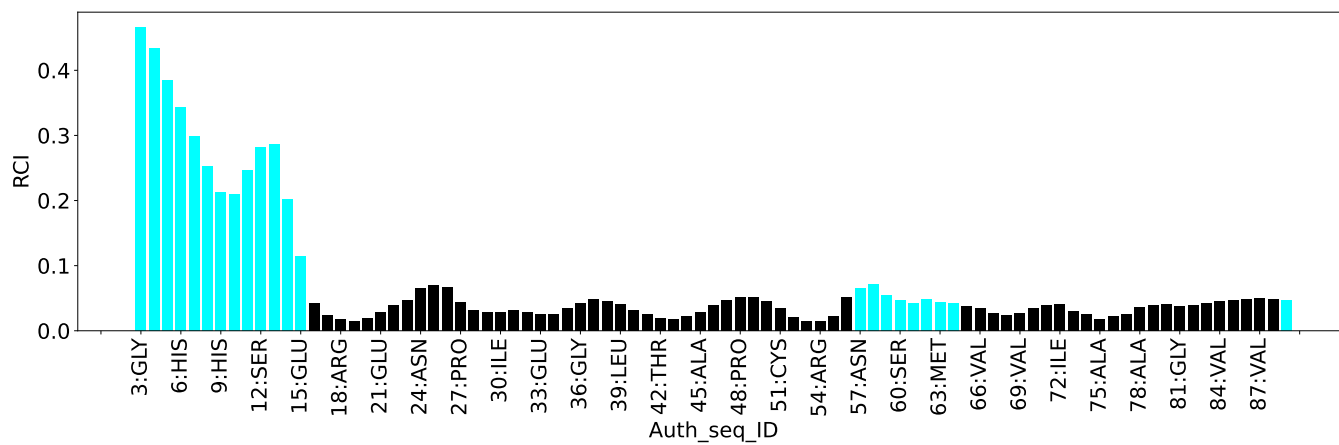
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 75  | ALA  | HA   | 1.75       | 2.13 – 6.34         | -5.9    |
| 1       | A     | 75  | ALA  | HB1  | -0.04      | 0.14 – 2.58         | -5.7    |
| 1       | A     | 75  | ALA  | HB2  | -0.04      | 0.14 – 2.58         | -5.7    |
| 1       | A     | 75  | ALA  | HB3  | -0.04      | 0.14 – 2.58         | -5.7    |

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

| Description  | Value |
|--|-------|
| Total distance restraints                                | 1023  |
| Intra-residue ( $ i-j =0$ )                              | 226   |
| Sequential ( $ i-j =1$ )                                 | 268   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 119   |
| Long range ( $ i-j \geq 5$ )                             | 410   |
| Inter-chain  | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 11.5  |
| Number of long range restraints per residue <sup>1</sup> | 4.6   |

<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)  | 15.3                                   | 0.2     |
| 0.2-0.5 (Medium) | 18.1                                   | 0.5     |
| >0.5 (Large)     | 13.3                                   | 2.4     |

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis [i](#)

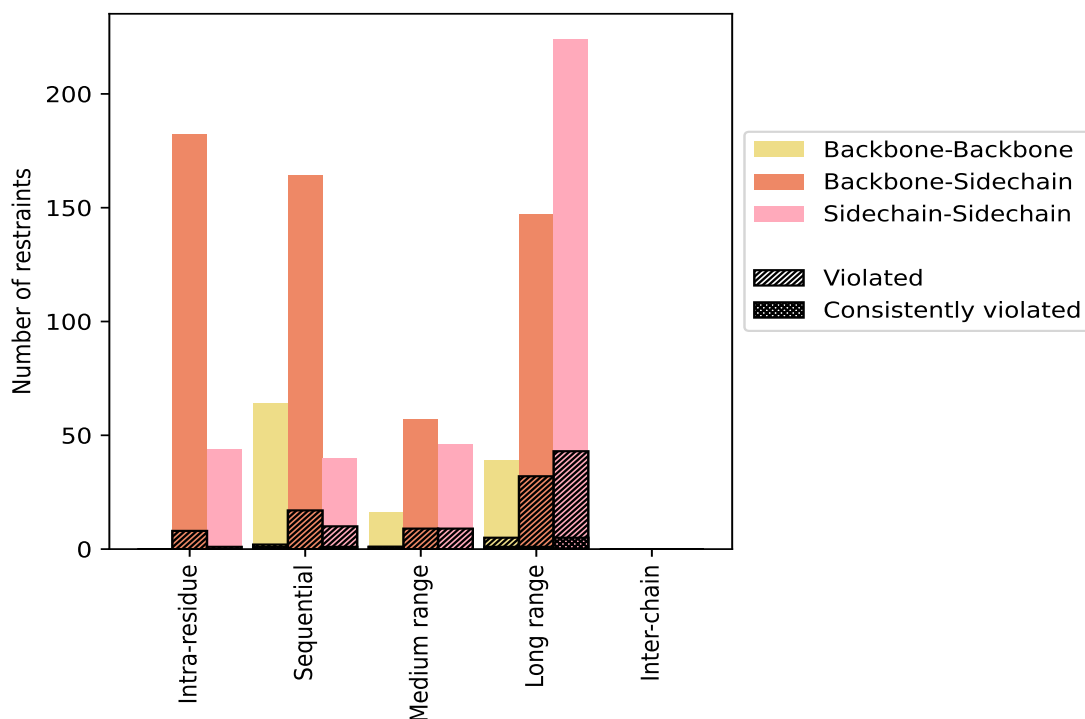
### 9.1 Summary of distance violations [i](#)

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

| Restrains type  | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|   |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>226</b>  | <b>22.1</b>    | <b>9</b>              | <b>4.0</b>     | <b>0.9</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 182         | 17.8           | 8                     | 4.4            | 0.8            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 44          | 4.3            | 1                     | 2.3            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>268</b>  | <b>26.2</b>    | <b>29</b>             | <b>10.8</b>    | <b>2.8</b>     | <b>2</b>                           | <b>0.7</b>     | <b>0.2</b>     |
| Backbone-Backbone   | 64          | 6.3            | 2                     | 3.1            | 0.2            | 1                                  | 1.6            | 0.1            |
| Backbone-Sidechain  | 164         | 16.0           | 17                    | 10.4           | 1.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 40          | 3.9            | 10                    | 25.0           | 1.0            | 1                                  | 2.5            | 0.1            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>119</b>  | <b>11.6</b>    | <b>19</b>             | <b>16.0</b>    | <b>1.9</b>     | <b>1</b>                           | <b>0.8</b>     | <b>0.1</b>     |
| Backbone-Backbone   | 16          | 1.6            | 1                     | 6.2            | 0.1            | 1                                  | 6.2            | 0.1            |
| Backbone-Sidechain  | 57          | 5.6            | 9                     | 15.8           | 0.9            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 46          | 4.5            | 9                     | 19.6           | 0.9            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>410</b>  | <b>40.1</b>    | <b>80</b>             | <b>19.5</b>    | <b>7.8</b>     | <b>7</b>                           | <b>1.7</b>     | <b>0.7</b>     |
| Backbone-Backbone   | 39          | 3.8            | 5                     | 12.8           | 0.5            | 1                                  | 2.6            | 0.1            |
| Backbone-Sidechain  | 147         | 14.4           | 32                    | 21.8           | 3.1            | 1                                  | 0.7            | 0.1            |
| Sidechain-Sidechain   | 224         | 21.9           | 43                    | 19.2           | 4.2            | 5                                  | 2.2            | 0.5            |
| <b>Inter-chain</b>  | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone   | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain  | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain   | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>  | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>   | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>  | <b>1023</b> | <b>100.0</b>   | <b>137</b>            | <b>13.4</b>    | <b>13.4</b>    | <b>10</b>                          | <b>1.0</b>     | <b>1.0</b>     |
| Backbone-Backbone   | 119         | 11.6           | 8                     | 6.7            | 0.8            | 3                                  | 2.5            | 0.3            |
| Backbone-Sidechain  | 550         | 53.8           | 66                    | 12.0           | 6.5            | 1                                  | 0.2            | 0.1            |
| Sidechain-Sidechain   | 354         | 34.6           | 63                    | 17.8           | 6.2            | 6                                  | 1.7            | 0.6            |

<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 disulfid 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        | 2                    | 10              | 4               | 46              | 0               | 62    | 0.58     | 2.4     | 0.52                | 0.38       |
| 2        | 2                    | 12              | 9               | 33              | 0               | 56    | 0.51     | 2.09    | 0.51                | 0.25       |
| 3        | 3                    | 9               | 7               | 31              | 0               | 50    | 0.55     | 2.26    | 0.54                | 0.29       |
| 4        | 2                    | 11              | 7               | 35              | 0               | 55    | 0.61     | 2.2     | 0.53                | 0.41       |
| 5        | 0                    | 8               | 4               | 28              | 0               | 40    | 0.38     | 1.67    | 0.34                | 0.22       |
| 6        | 2                    | 9               | 4               | 28              | 0               | 43    | 0.39     | 1.37    | 0.32                | 0.23       |
| 7        | 2                    | 8               | 6               | 31              | 0               | 47    | 0.39     | 1.42    | 0.31                | 0.26       |
| 8        | 2                    | 5               | 5               | 27              | 0               | 39    | 0.42     | 1.67    | 0.36                | 0.28       |
| 9        | 1                    | 9               | 5               | 35              | 0               | 50    | 0.53     | 1.86    | 0.49                | 0.29       |
| 10       | 2                    | 10              | 4               | 30              | 0               | 46    | 0.63     | 2.33    | 0.55                | 0.42       |
| 11       | 2                    | 11              | 10              | 27              | 0               | 50    | 0.36     | 1.55    | 0.32                | 0.23       |

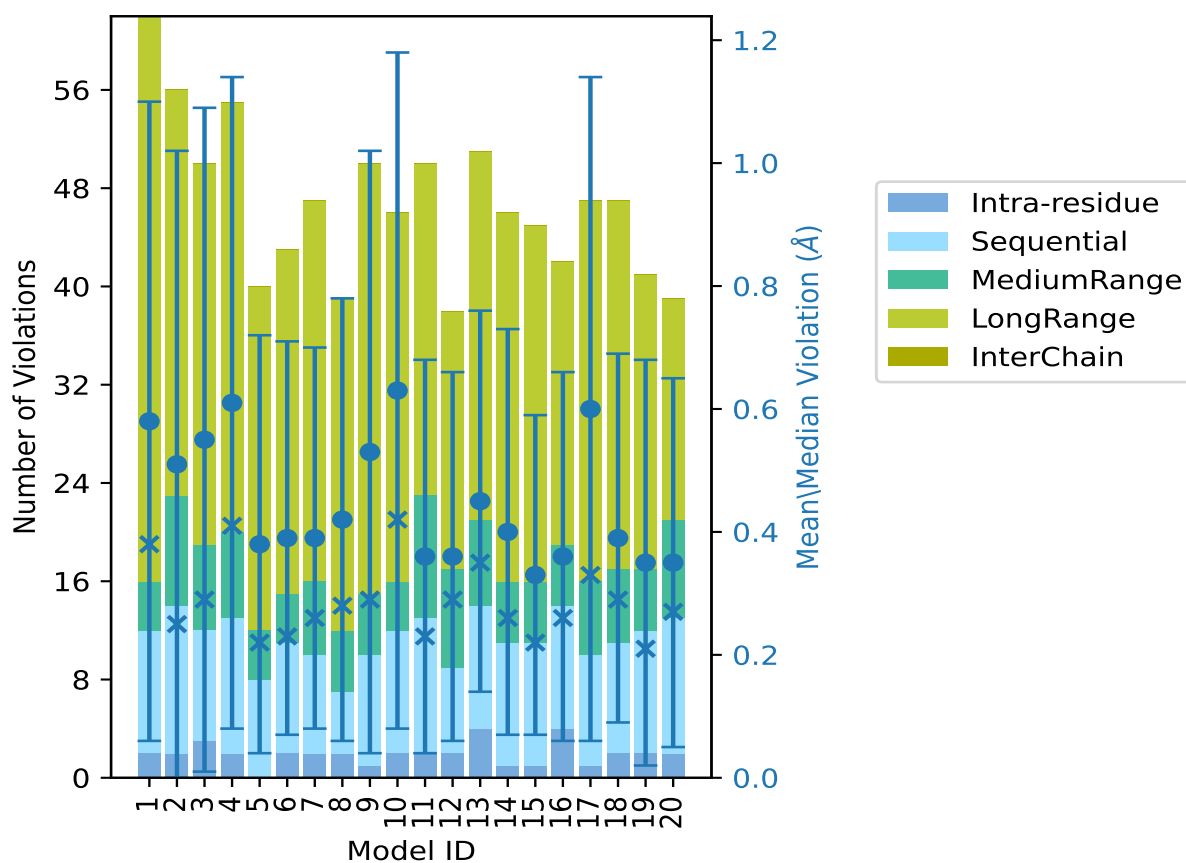
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| Model ID | Number of violations |                 |                 |                 |                 | Total | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> |       |          |         |                     |            |
| 12       | 2                    | 7               | 8               | 21              | 0               | 38    | 0.36     | 1.72    | 0.3                 | 0.29       |
| 13       | 4                    | 10              | 7               | 30              | 0               | 51    | 0.45     | 1.27    | 0.31                | 0.35       |
| 14       | 1                    | 10              | 5               | 30              | 0               | 46    | 0.4      | 1.49    | 0.33                | 0.26       |
| 15       | 1                    | 10              | 5               | 29              | 0               | 45    | 0.33     | 1.23    | 0.26                | 0.22       |
| 16       | 4                    | 10              | 5               | 23              | 0               | 42    | 0.36     | 1.69    | 0.3                 | 0.26       |
| 17       | 1                    | 9               | 6               | 31              | 0               | 47    | 0.6      | 2.25    | 0.54                | 0.33       |
| 18       | 2                    | 9               | 6               | 30              | 0               | 47    | 0.39     | 1.36    | 0.3                 | 0.29       |
| 19       | 2                    | 10              | 5               | 24              | 0               | 41    | 0.35     | 1.8     | 0.33                | 0.21       |
| 20       | 2                    | 11              | 8               | 18              | 0               | 39    | 0.35     | 1.64    | 0.3                 | 0.27       |

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

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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



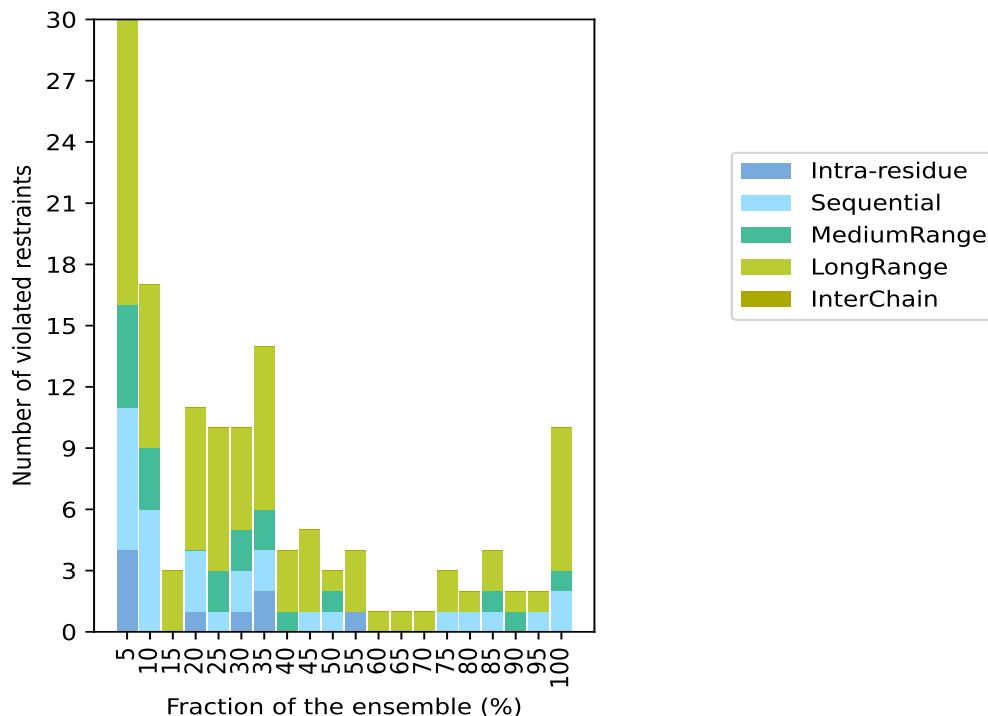
### 9.3 Distance violation statistics for the ensemble

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, 886(IR:217, SQ:239, MR:100, LR:330, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 4                             | 7               | 5               | 14              | 0               | 30    | 1                        | 5.0   |
| 0                             | 6               | 3               | 8               | 0               | 17    | 2                        | 10.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 3                        | 15.0  |
| 1                             | 3               | 0               | 7               | 0               | 11    | 4                        | 20.0  |
| 0                             | 1               | 2               | 7               | 0               | 10    | 5                        | 25.0  |
| 1                             | 2               | 2               | 5               | 0               | 10    | 6                        | 30.0  |
| 2                             | 2               | 2               | 8               | 0               | 14    | 7                        | 35.0  |
| 0                             | 0               | 1               | 3               | 0               | 4     | 8                        | 40.0  |
| 0                             | 1               | 0               | 4               | 0               | 5     | 9                        | 45.0  |
| 0                             | 1               | 1               | 1               | 0               | 3     | 10                       | 50.0  |
| 1                             | 0               | 0               | 3               | 0               | 4     | 11                       | 55.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 12                       | 60.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 14                       | 70.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 15                       | 75.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 16                       | 80.0  |
| 0                             | 1               | 1               | 2               | 0               | 4     | 17                       | 85.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 18                       | 90.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 19                       | 95.0  |
| 0                             | 2               | 1               | 7               | 0               | 10    | 20                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

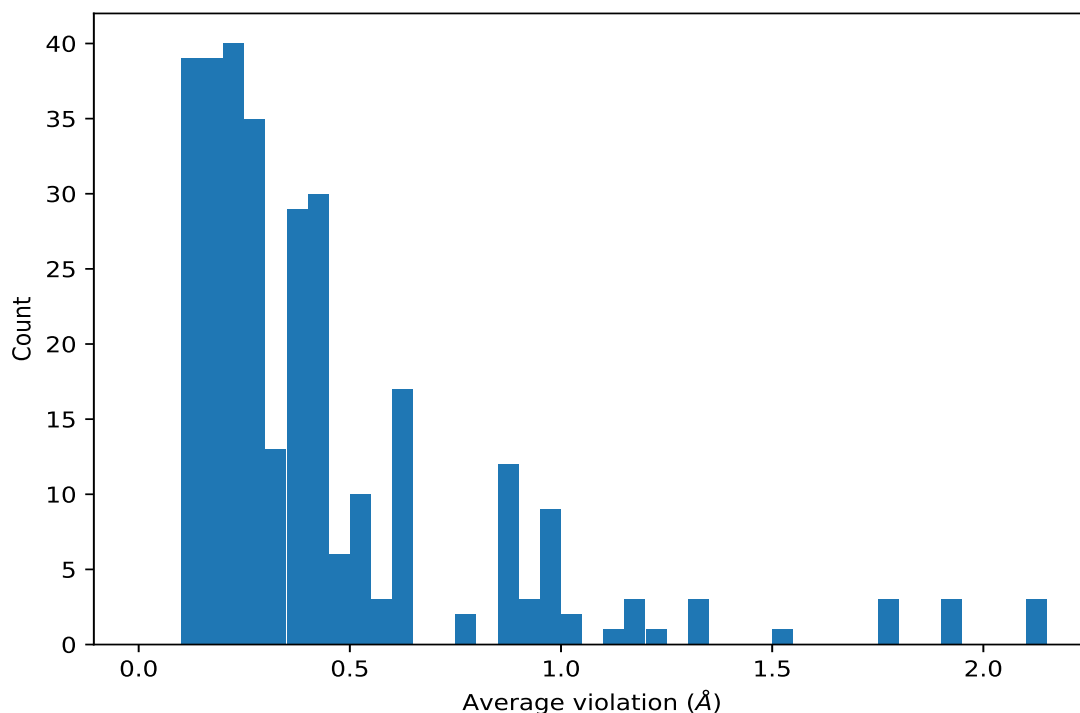
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,464) | 1:A:15:GLU:H    | 1:A:36:GLY:HA3  | 20                  | 1.53     | 0.23                | 1.63       |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 20                  | 1.21     | 0.03                | 1.2        |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 20                  | 0.77     | 0.35                | 0.69       |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 20                  | 0.64     | 0.08                | 0.66       |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 20                  | 0.53     | 0.18                | 0.49       |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 20                  | 0.37     | 0.13                | 0.4        |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 20                  | 0.37     | 0.13                | 0.4        |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 20                  | 0.36     | 0.07                | 0.34       |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 20                  | 0.36     | 0.07                | 0.34       |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 20                  | 0.36     | 0.07                | 0.34       |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 20                  | 0.36     | 0.07                | 0.34       |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 20                  | 0.36     | 0.07                | 0.34       |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 20                  | 0.36     | 0.07                | 0.34       |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 20                  | 0.36     | 0.07                | 0.34       |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 20                  | 0.36     | 0.07                | 0.34       |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 20                  | 0.36     | 0.07                | 0.34       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 20                  | 0.31     | 0.21                | 0.17       |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 20                  | 0.31     | 0.21                | 0.17       |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 20                  | 0.31     | 0.21                | 0.17       |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 20                  | 0.27     | 0.07                | 0.26       |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 20                  | 0.27     | 0.07                | 0.26       |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 20                  | 0.27     | 0.07                | 0.26       |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 20                  | 0.17     | 0.05                | 0.15       |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 19                  | 0.26     | 0.06                | 0.28       |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 19                  | 0.2      | 0.01                | 0.2        |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 18                  | 0.21     | 0.06                | 0.2        |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 18                  | 0.21     | 0.06                | 0.2        |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 18                  | 0.21     | 0.06                | 0.2        |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 18                  | 0.21     | 0.06                | 0.2        |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 18                  | 0.21     | 0.06                | 0.2        |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 18                  | 0.21     | 0.06                | 0.2        |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 18                  | 0.2      | 0.02                | 0.21       |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 18                  | 0.2      | 0.02                | 0.21       |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 18                  | 0.2      | 0.02                | 0.21       |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 17                  | 0.78     | 0.36                | 0.86       |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 17                  | 0.26     | 0.13                | 0.23       |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 17                  | 0.26     | 0.13                | 0.23       |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 17                  | 0.2      | 0.08                | 0.18       |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 17                  | 0.15     | 0.05                | 0.13       |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 16                  | 0.37     | 0.15                | 0.38       |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 16                  | 0.37     | 0.15                | 0.38       |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 16                  | 0.23     | 0.04                | 0.23       |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 16                  | 0.23     | 0.04                | 0.23       |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 16                  | 0.23     | 0.04                | 0.23       |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 16                  | 0.23     | 0.04                | 0.23       |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 16                  | 0.23     | 0.04                | 0.23       |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 16                  | 0.23     | 0.04                | 0.23       |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 15                  | 0.55     | 0.24                | 0.48       |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 15                  | 0.36     | 0.23                | 0.25       |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 15                  | 0.36     | 0.23                | 0.25       |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 15                  | 0.36     | 0.23                | 0.25       |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 15                  | 0.36     | 0.28                | 0.16       |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 14                  | 0.31     | 0.15                | 0.28       |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 13                  | 0.36     | 0.18                | 0.3        |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 13                  | 0.36     | 0.18                | 0.3        |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 13                  | 0.36     | 0.18                | 0.3        |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 12                  | 0.2      | 0.05                | 0.18       |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 11                  | 0.48     | 0.14                | 0.56       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 11                  | 0.3      | 0.16                | 0.32       |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 11                  | 0.3      | 0.16                | 0.32       |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 11                  | 0.3      | 0.16                | 0.32       |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 11                  | 0.21     | 0.01                | 0.21       |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 11                  | 0.19     | 0.05                | 0.19       |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 10                  | 0.64     | 0.33                | 0.8        |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2  | 10                  | 0.49     | 0.34                | 0.4        |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB   | 10                  | 0.17     | 0.04                | 0.18       |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB   | 9                   | 0.57     | 0.37                | 0.47       |
| (1,749) | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 9                   | 0.3      | 0.2                 | 0.26       |
| (1,642) | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3  | 9                   | 0.26     | 0.05                | 0.27       |
| (1,642) | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3  | 9                   | 0.26     | 0.05                | 0.27       |
| (1,642) | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3  | 9                   | 0.26     | 0.05                | 0.27       |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 9                   | 0.22     | 0.06                | 0.25       |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 9                   | 0.22     | 0.06                | 0.25       |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 9                   | 0.19     | 0.04                | 0.21       |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 9                   | 0.19     | 0.04                | 0.21       |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 9                   | 0.19     | 0.04                | 0.21       |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 9                   | 0.19     | 0.04                | 0.21       |
| (1,318) | 1:A:21:GLU:HA   | 1:A:87:VAL:HG11 | 8                   | 1.94     | 0.69                | 2.22       |
| (1,318) | 1:A:21:GLU:HA   | 1:A:87:VAL:HG12 | 8                   | 1.94     | 0.69                | 2.22       |
| (1,318) | 1:A:21:GLU:HA   | 1:A:87:VAL:HG13 | 8                   | 1.94     | 0.69                | 2.22       |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 8                   | 0.42     | 0.22                | 0.55       |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 8                   | 0.42     | 0.22                | 0.55       |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 8                   | 0.42     | 0.22                | 0.55       |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 8                   | 0.42     | 0.22                | 0.55       |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 8                   | 0.42     | 0.22                | 0.55       |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 8                   | 0.42     | 0.22                | 0.55       |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 8                   | 0.34     | 0.14                | 0.39       |
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 8                   | 0.34     | 0.14                | 0.39       |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA   | 8                   | 0.28     | 0.08                | 0.31       |
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 8                   | 0.28     | 0.08                | 0.31       |
| (1,60)  | 1:A:21:GLU:H    | 1:A:87:VAL:HG11 | 7                   | 2.1      | 0.15                | 2.15       |
| (1,60)  | 1:A:21:GLU:H    | 1:A:87:VAL:HG12 | 7                   | 2.1      | 0.15                | 2.15       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,60)  | 1:A:21:GLU:H    | 1:A:87:VAL:HG13 | 7                   | 2.1      | 0.15                | 2.15       |
| (1,735) | 1:A:21:GLU:HB2  | 1:A:87:VAL:HG11 | 7                   | 1.79     | 0.18                | 1.73       |
| (1,735) | 1:A:21:GLU:HB2  | 1:A:87:VAL:HG12 | 7                   | 1.79     | 0.18                | 1.73       |
| (1,735) | 1:A:21:GLU:HB2  | 1:A:87:VAL:HG13 | 7                   | 1.79     | 0.18                | 1.73       |
| (1,321) | 1:A:86:VAL:HA   | 1:A:87:VAL:HG11 | 7                   | 1.34     | 0.03                | 1.35       |
| (1,321) | 1:A:86:VAL:HA   | 1:A:87:VAL:HG12 | 7                   | 1.34     | 0.03                | 1.35       |
| (1,321) | 1:A:86:VAL:HA   | 1:A:87:VAL:HG13 | 7                   | 1.34     | 0.03                | 1.35       |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG11 | 7                   | 1.19     | 0.34                | 1.44       |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG12 | 7                   | 1.19     | 0.34                | 1.44       |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG13 | 7                   | 1.19     | 0.34                | 1.44       |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG11 | 7                   | 0.99     | 0.28                | 1.02       |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG12 | 7                   | 0.99     | 0.28                | 1.02       |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG13 | 7                   | 0.99     | 0.28                | 1.02       |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG11 | 7                   | 0.95     | 0.09                | 0.98       |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG12 | 7                   | 0.95     | 0.09                | 0.98       |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG13 | 7                   | 0.95     | 0.09                | 0.98       |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG11 | 7                   | 0.95     | 0.09                | 0.98       |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG12 | 7                   | 0.95     | 0.09                | 0.98       |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG13 | 7                   | 0.95     | 0.09                | 0.98       |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG11 | 7                   | 0.92     | 0.01                | 0.92       |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG12 | 7                   | 0.92     | 0.01                | 0.92       |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG13 | 7                   | 0.92     | 0.01                | 0.92       |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG11 | 7                   | 0.88     | 0.15                | 0.91       |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG12 | 7                   | 0.88     | 0.15                | 0.91       |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG13 | 7                   | 0.88     | 0.15                | 0.91       |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG11 | 7                   | 0.88     | 0.15                | 0.91       |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG12 | 7                   | 0.88     | 0.15                | 0.91       |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG13 | 7                   | 0.88     | 0.15                | 0.91       |
| (1,503) | 1:A:75:ALA:HB1  | 1:A:80:TRP:HE3  | 7                   | 0.43     | 0.03                | 0.42       |
| (1,503) | 1:A:75:ALA:HB2  | 1:A:80:TRP:HE3  | 7                   | 0.43     | 0.03                | 0.42       |
| (1,503) | 1:A:75:ALA:HB3  | 1:A:80:TRP:HE3  | 7                   | 0.43     | 0.03                | 0.42       |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB1  | 7                   | 0.29     | 0.11                | 0.27       |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB2  | 7                   | 0.29     | 0.11                | 0.27       |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB3  | 7                   | 0.29     | 0.11                | 0.27       |
| (1,625) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HA   | 7                   | 0.22     | 0.05                | 0.24       |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD1  | 7                   | 0.18     | 0.04                | 0.18       |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD2  | 7                   | 0.18     | 0.04                | 0.18       |
| (1,163) | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE1  | 7                   | 0.17     | 0.04                | 0.18       |
| (1,163) | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE2  | 7                   | 0.17     | 0.04                | 0.18       |
| (1,556) | 1:A:40:LEU:HB3  | 1:A:41:SER:HA   | 7                   | 0.14     | 0.02                | 0.13       |
| (1,627) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HA   | 6                   | 0.55     | 0.23                | 0.55       |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB1  | 6                   | 0.52     | 0.07                | 0.55       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB2  | 6                   | 0.52     | 0.07                | 0.55       |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB3  | 6                   | 0.52     | 0.07                | 0.55       |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB1  | 6                   | 0.52     | 0.07                | 0.55       |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB2  | 6                   | 0.52     | 0.07                | 0.55       |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB3  | 6                   | 0.52     | 0.07                | 0.55       |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB1  | 6                   | 0.52     | 0.07                | 0.55       |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB2  | 6                   | 0.52     | 0.07                | 0.55       |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB3  | 6                   | 0.52     | 0.07                | 0.55       |
| (1,691) | 1:A:40:LEU:HB2  | 1:A:40:LEU:HG   | 6                   | 0.48     | 0.0                 | 0.48       |
| (1,314) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 6                   | 0.4      | 0.02                | 0.4        |
| (1,314) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 6                   | 0.4      | 0.02                | 0.4        |
| (1,314) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 6                   | 0.4      | 0.02                | 0.4        |
| (1,874) | 1:A:40:LEU:HD11 | 1:A:41:SER:HA   | 6                   | 0.36     | 0.04                | 0.38       |
| (1,874) | 1:A:40:LEU:HD12 | 1:A:41:SER:HA   | 6                   | 0.36     | 0.04                | 0.38       |
| (1,874) | 1:A:40:LEU:HD13 | 1:A:41:SER:HA   | 6                   | 0.36     | 0.04                | 0.38       |
| (1,874) | 1:A:40:LEU:HD21 | 1:A:41:SER:HA   | 6                   | 0.36     | 0.04                | 0.38       |
| (1,874) | 1:A:40:LEU:HD22 | 1:A:41:SER:HA   | 6                   | 0.36     | 0.04                | 0.38       |
| (1,874) | 1:A:40:LEU:HD23 | 1:A:41:SER:HA   | 6                   | 0.36     | 0.04                | 0.38       |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG11 | 6                   | 0.33     | 0.1                 | 0.32       |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG12 | 6                   | 0.33     | 0.1                 | 0.32       |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG13 | 6                   | 0.33     | 0.1                 | 0.32       |
| (1,693) | 1:A:30:ILE:HB   | 1:A:46:GLN:HG2  | 6                   | 0.28     | 0.04                | 0.27       |
| (1,480) | 1:A:75:ALA:HB1  | 1:A:79:GLY:H    | 6                   | 0.27     | 0.01                | 0.28       |
| (1,480) | 1:A:75:ALA:HB2  | 1:A:79:GLY:H    | 6                   | 0.27     | 0.01                | 0.28       |
| (1,480) | 1:A:75:ALA:HB3  | 1:A:79:GLY:H    | 6                   | 0.27     | 0.01                | 0.28       |
| (1,746) | 1:A:40:LEU:HA   | 1:A:71:GLY:HA3  | 6                   | 0.2      | 0.07                | 0.19       |
| (1,354) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HB2  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,354) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HB3  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,354) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB2  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,354) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB3  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,354) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB2  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,354) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB3  | 6                   | 0.16     | 0.01                | 0.16       |
| (1,529) | 1:A:55:TYR:HA   | 1:A:83:LEU:HG   | 5                   | 0.88     | 0.07                | 0.84       |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB1  | 5                   | 0.41     | 0.17                | 0.41       |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB2  | 5                   | 0.41     | 0.17                | 0.41       |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB3  | 5                   | 0.41     | 0.17                | 0.41       |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB1  | 5                   | 0.41     | 0.17                | 0.41       |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB2  | 5                   | 0.41     | 0.17                | 0.41       |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB3  | 5                   | 0.41     | 0.17                | 0.41       |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB1  | 5                   | 0.41     | 0.17                | 0.41       |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB2  | 5                   | 0.41     | 0.17                | 0.41       |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB3  | 5                   | 0.41     | 0.17                | 0.41       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,492) | 1:A:50:ALA:HB1  | 1:A:52:GLY:H    | 5                   | 0.4      | 0.15                | 0.47       |
| (1,492) | 1:A:50:ALA:HB2  | 1:A:52:GLY:H    | 5                   | 0.4      | 0.15                | 0.47       |
| (1,492) | 1:A:50:ALA:HB3  | 1:A:52:GLY:H    | 5                   | 0.4      | 0.15                | 0.47       |
| (1,896) | 1:A:53:LEU:HD11 | 1:A:73:LEU:HB3  | 5                   | 0.28     | 0.01                | 0.28       |
| (1,896) | 1:A:53:LEU:HD12 | 1:A:73:LEU:HB3  | 5                   | 0.28     | 0.01                | 0.28       |
| (1,896) | 1:A:53:LEU:HD13 | 1:A:73:LEU:HB3  | 5                   | 0.28     | 0.01                | 0.28       |
| (1,896) | 1:A:53:LEU:HD21 | 1:A:73:LEU:HB3  | 5                   | 0.28     | 0.01                | 0.28       |
| (1,896) | 1:A:53:LEU:HD22 | 1:A:73:LEU:HB3  | 5                   | 0.28     | 0.01                | 0.28       |
| (1,896) | 1:A:53:LEU:HD23 | 1:A:73:LEU:HB3  | 5                   | 0.28     | 0.01                | 0.28       |
| (1,131) | 1:A:55:TYR:HD1  | 1:A:83:LEU:HG   | 5                   | 0.26     | 0.02                | 0.26       |
| (1,131) | 1:A:55:TYR:HD2  | 1:A:83:LEU:HG   | 5                   | 0.26     | 0.02                | 0.26       |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB1  | 5                   | 0.18     | 0.04                | 0.2        |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB2  | 5                   | 0.18     | 0.04                | 0.2        |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB3  | 5                   | 0.18     | 0.04                | 0.2        |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB1  | 5                   | 0.17     | 0.05                | 0.13       |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB2  | 5                   | 0.17     | 0.05                | 0.13       |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB3  | 5                   | 0.17     | 0.05                | 0.13       |
| (1,668) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HD3  | 5                   | 0.14     | 0.01                | 0.14       |
| (1,668) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HD3  | 5                   | 0.14     | 0.01                | 0.14       |
| (1,668) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HD3  | 5                   | 0.14     | 0.01                | 0.14       |
| (1,323) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 5                   | 0.14     | 0.01                | 0.13       |
| (1,323) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 5                   | 0.14     | 0.01                | 0.13       |
| (1,323) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 5                   | 0.14     | 0.01                | 0.13       |
| (1,569) | 1:A:52:GLY:HA3  | 1:A:88:ASN:H    | 5                   | 0.13     | 0.01                | 0.12       |
| (1,184) | 1:A:32:SER:HB2  | 1:A:80:TRP:HZ2  | 4                   | 1.12     | 0.08                | 1.14       |
| (1,759) | 1:A:32:SER:HB2  | 1:A:39:LEU:H    | 4                   | 1.02     | 0.13                | 1.03       |
| (1,644) | 1:A:31:PRO:HA   | 1:A:32:SER:HB3  | 4                   | 1.01     | 0.01                | 1.0        |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG11 | 4                   | 0.86     | 0.06                | 0.86       |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG12 | 4                   | 0.86     | 0.06                | 0.86       |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG13 | 4                   | 0.86     | 0.06                | 0.86       |
| (1,108) | 1:A:6:HIS:H     | 1:A:6:HIS:HD2   | 4                   | 0.6      | 0.17                | 0.56       |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD11 | 4                   | 0.25     | 0.08                | 0.26       |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD12 | 4                   | 0.25     | 0.08                | 0.26       |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD13 | 4                   | 0.25     | 0.08                | 0.26       |
| (1,496) | 1:A:32:SER:HB3  | 1:A:80:TRP:HD1  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD11 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD12 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD13 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD21 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD22 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD23 | 4                   | 0.2      | 0.01                | 0.2        |
| (1,135) | 1:A:53:LEU:HG   | 1:A:85:TYR:HE1  | 4                   | 0.17     | 0.01                | 0.18       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,135) | 1:A:53:LEU:HG   | 1:A:85:TYR:HE2  | 4                   | 0.17     | 0.01                | 0.18       |
| (1,967) | 1:A:66:VAL:HG11 | 1:A:85:TYR:HA   | 4                   | 0.17     | 0.04                | 0.15       |
| (1,967) | 1:A:66:VAL:HG12 | 1:A:85:TYR:HA   | 4                   | 0.17     | 0.04                | 0.15       |
| (1,967) | 1:A:66:VAL:HG13 | 1:A:85:TYR:HA   | 4                   | 0.17     | 0.04                | 0.15       |
| (1,967) | 1:A:66:VAL:HG21 | 1:A:85:TYR:HA   | 4                   | 0.17     | 0.04                | 0.15       |
| (1,967) | 1:A:66:VAL:HG22 | 1:A:85:TYR:HA   | 4                   | 0.17     | 0.04                | 0.15       |
| (1,967) | 1:A:66:VAL:HG23 | 1:A:85:TYR:HA   | 4                   | 0.17     | 0.04                | 0.15       |
| (1,643) | 1:A:17:ILE:HG21 | 1:A:32:SER:HB3  | 4                   | 0.13     | 0.01                | 0.12       |
| (1,643) | 1:A:17:ILE:HG22 | 1:A:32:SER:HB3  | 4                   | 0.13     | 0.01                | 0.12       |
| (1,643) | 1:A:17:ILE:HG23 | 1:A:32:SER:HB3  | 4                   | 0.13     | 0.01                | 0.12       |
| (1,303) | 1:A:28:ILE:HG21 | 1:A:46:GLN:HG3  | 3                   | 0.37     | 0.15                | 0.45       |
| (1,303) | 1:A:28:ILE:HG22 | 1:A:46:GLN:HG3  | 3                   | 0.37     | 0.15                | 0.45       |
| (1,303) | 1:A:28:ILE:HG23 | 1:A:46:GLN:HG3  | 3                   | 0.37     | 0.15                | 0.45       |
| (1,790) | 1:A:15:GLU:HB2  | 1:A:36:GLY:HA3  | 3                   | 0.24     | 0.05                | 0.24       |
| (1,790) | 1:A:15:GLU:HB3  | 1:A:36:GLY:HA3  | 3                   | 0.24     | 0.05                | 0.24       |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG11 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG12 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG13 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG21 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG22 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG23 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG11 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG12 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG13 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG21 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG22 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG23 | 3                   | 0.14     | 0.02                | 0.15       |
| (1,890) | 1:A:53:LEU:H    | 1:A:88:ASN:HB2  | 2                   | 0.89     | 0.01                | 0.89       |
| (1,890) | 1:A:53:LEU:H    | 1:A:88:ASN:HB3  | 2                   | 0.89     | 0.01                | 0.89       |
| (1,626) | 1:A:13:MET:HG2  | 1:A:14:SER:HB2  | 2                   | 0.64     | 0.03                | 0.64       |
| (1,626) | 1:A:13:MET:HG2  | 1:A:14:SER:HB3  | 2                   | 0.64     | 0.03                | 0.64       |
| (1,626) | 1:A:13:MET:HG3  | 1:A:14:SER:HB2  | 2                   | 0.64     | 0.03                | 0.64       |
| (1,626) | 1:A:13:MET:HG3  | 1:A:14:SER:HB3  | 2                   | 0.64     | 0.03                | 0.64       |
| (1,632) | 1:A:54:ARG:HG3  | 1:A:65:GLY:HA2  | 2                   | 0.62     | 0.18                | 0.62       |
| (1,632) | 1:A:54:ARG:HG3  | 1:A:65:GLY:HA3  | 2                   | 0.62     | 0.18                | 0.62       |
| (1,663) | 1:A:45:ALA:HB1  | 1:A:46:GLN:HG2  | 2                   | 0.46     | 0.1                 | 0.46       |
| (1,663) | 1:A:45:ALA:HB2  | 1:A:46:GLN:HG2  | 2                   | 0.46     | 0.1                 | 0.46       |
| (1,663) | 1:A:45:ALA:HB3  | 1:A:46:GLN:HG2  | 2                   | 0.46     | 0.1                 | 0.46       |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG11 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG12 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG13 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG21 | 2                   | 0.44     | 0.3                 | 0.44       |

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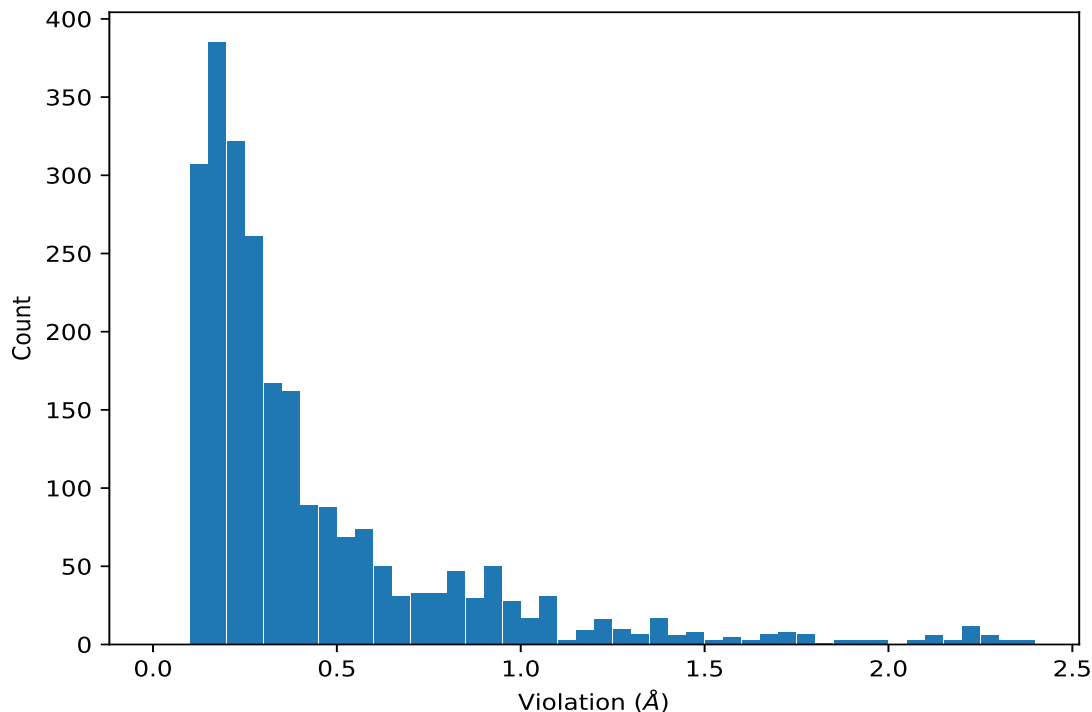
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,815)  | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG22 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,815)  | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG23 | 2                   | 0.44     | 0.3                 | 0.44       |
| (1,672)  | 1:A:69:VAL:HG21 | 1:A:70:GLU:HG2  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,672)  | 1:A:69:VAL:HG21 | 1:A:70:GLU:HG3  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,672)  | 1:A:69:VAL:HG22 | 1:A:70:GLU:HG2  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,672)  | 1:A:69:VAL:HG22 | 1:A:70:GLU:HG3  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,672)  | 1:A:69:VAL:HG23 | 1:A:70:GLU:HG2  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,672)  | 1:A:69:VAL:HG23 | 1:A:70:GLU:HG3  | 2                   | 0.26     | 0.01                | 0.26       |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD11 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD12 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD13 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD11 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD12 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD13 | 2                   | 0.23     | 0.05                | 0.23       |
| (1,888)  | 1:A:52:GLY:HA3  | 1:A:88:ASN:HB2  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,888)  | 1:A:52:GLY:HA3  | 1:A:88:ASN:HB3  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,840)  | 1:A:33:GLU:HB2  | 1:A:39:LEU:H    | 2                   | 0.18     | 0.02                | 0.18       |
| (1,840)  | 1:A:33:GLU:HB3  | 1:A:39:LEU:H    | 2                   | 0.18     | 0.02                | 0.18       |
| (1,688)  | 1:A:40:LEU:HB2  | 1:A:43:VAL:HG21 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,688)  | 1:A:40:LEU:HB2  | 1:A:43:VAL:HG22 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,688)  | 1:A:40:LEU:HB2  | 1:A:43:VAL:HG23 | 2                   | 0.17     | 0.02                | 0.17       |
| (1,938)  | 1:A:57:ASN:HD21 | 1:A:60:SER:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,938)  | 1:A:57:ASN:HD22 | 1:A:60:SER:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,885)  | 1:A:52:GLY:H    | 1:A:88:ASN:HB2  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,885)  | 1:A:52:GLY:H    | 1:A:88:ASN:HB3  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,391)  | 1:A:33:GLU:H    | 1:A:38:VAL:HG11 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,391)  | 1:A:33:GLU:H    | 1:A:38:VAL:HG12 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,391)  | 1:A:33:GLU:H    | 1:A:38:VAL:HG13 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1019) | 1:A:87:VAL:HA   | 1:A:88:ASN:HB2  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1019) | 1:A:87:VAL:HA   | 1:A:88:ASN:HB3  | 2                   | 0.14     | 0.02                | 0.14       |
| (1,455)  | 1:A:55:TYR:HA   | 1:A:66:VAL:H    | 2                   | 0.13     | 0.0                 | 0.13       |
| (1,841)  | 1:A:35:ASP:HB2  | 1:A:36:GLY:HA3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,841)  | 1:A:35:ASP:HB3  | 1:A:36:GLY:HA3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG11 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG12 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG13 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG21 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG23 | 2                   | 0.12     | 0.0                 | 0.12       |

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

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

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

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



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

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

| Key     | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|---------|---------------|-----------------|----------|---------------|
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG11 | 1        | 2.4           |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG12 | 1        | 2.4           |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG13 | 1        | 2.4           |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG11 | 10       | 2.33          |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG12 | 10       | 2.33          |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG13 | 10       | 2.33          |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG11 | 3        | 2.26          |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG12 | 3        | 2.26          |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG13 | 3        | 2.26          |
| (1,318) | 1:A:21:GLU:HA | 1:A:87:VAL:HG11 | 17       | 2.25          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG12 | 17       | 2.25          |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG13 | 17       | 2.25          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG11 | 1        | 2.22          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG12 | 1        | 2.22          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG13 | 1        | 2.22          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG11 | 10       | 2.21          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG12 | 10       | 2.21          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG13 | 10       | 2.21          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG11 | 17       | 2.2           |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG12 | 17       | 2.2           |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG13 | 17       | 2.2           |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG11 | 4        | 2.2           |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG12 | 4        | 2.2           |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG13 | 4        | 2.2           |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG11 | 4        | 2.15          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG12 | 4        | 2.15          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG13 | 4        | 2.15          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG11 | 3        | 2.14          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG12 | 3        | 2.14          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG13 | 3        | 2.14          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG11 | 4        | 2.13          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG12 | 4        | 2.13          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG13 | 4        | 2.13          |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG11 | 2        | 2.09          |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG12 | 2        | 2.09          |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG13 | 2        | 2.09          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG11 | 2        | 1.99          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG12 | 2        | 1.99          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG13 | 2        | 1.99          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG11 | 2        | 1.91          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG12 | 2        | 1.91          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG13 | 2        | 1.91          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG11 | 9        | 1.86          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG12 | 9        | 1.86          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG13 | 9        | 1.86          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 19       | 1.8           |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG11 | 9        | 1.79          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG12 | 9        | 1.79          |
| (1,60)  | 1:A:21:GLU:H   | 1:A:87:VAL:HG13 | 9        | 1.79          |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG11 | 9        | 1.79          |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG12 | 9        | 1.79          |
| (1,318) | 1:A:21:GLU:HA  | 1:A:87:VAL:HG13 | 9        | 1.79          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 1        | 1.75          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG11 | 3        | 1.73          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG12 | 3        | 1.73          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG13 | 3        | 1.73          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG11 | 1        | 1.72          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG12 | 1        | 1.72          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG13 | 1        | 1.72          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 12       | 1.72          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 3        | 1.71          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 16       | 1.69          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 2        | 1.67          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 5        | 1.67          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 8        | 1.67          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG11 | 17       | 1.65          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG12 | 17       | 1.65          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG13 | 17       | 1.65          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 9        | 1.64          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 20       | 1.64          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 10       | 1.63          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG11 | 10       | 1.56          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG12 | 10       | 1.56          |
| (1,735) | 1:A:21:GLU:HB2 | 1:A:87:VAL:HG13 | 10       | 1.56          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 4        | 1.56          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 11       | 1.55          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG11 | 17       | 1.54          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG12 | 17       | 1.54          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG13 | 17       | 1.54          |
| (1,653) | 1:A:21:GLU:HB2 | 1:A:47:PHE:HB3  | 9        | 1.49          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 14       | 1.49          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG11 | 10       | 1.49          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG12 | 10       | 1.49          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG13 | 10       | 1.49          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG11 | 1        | 1.46          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG12 | 1        | 1.46          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG13 | 1        | 1.46          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG11 | 3        | 1.44          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG12 | 3        | 1.44          |
| (1,309) | 1:A:21:GLU:HB3 | 1:A:87:VAL:HG13 | 3        | 1.44          |
| (1,653) | 1:A:21:GLU:HB2 | 1:A:47:PHE:HB3  | 4        | 1.42          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 7        | 1.42          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 17       | 1.42          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG11 | 17       | 1.39          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG12 | 17       | 1.39          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG13 | 17       | 1.39          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 6        | 1.37          |
| (1,653) | 1:A:21:GLU:HB2 | 1:A:47:PHE:HB3  | 18       | 1.36          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG11 | 4        | 1.36          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG12 | 4        | 1.36          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG13 | 4        | 1.36          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG11 | 10       | 1.36          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG12 | 10       | 1.36          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG13 | 10       | 1.36          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG11 | 2        | 1.35          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG12 | 2        | 1.35          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG13 | 2        | 1.35          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG11 | 3        | 1.35          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG12 | 3        | 1.35          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG13 | 3        | 1.35          |
| (1,653) | 1:A:21:GLU:HB2 | 1:A:47:PHE:HB3  | 2        | 1.31          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG11 | 1        | 1.31          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG12 | 1        | 1.31          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG13 | 1        | 1.31          |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG11 | 10       | 1.3           |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG12 | 10       | 1.3           |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG13 | 10       | 1.3           |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG11 | 9        | 1.29          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG12 | 9        | 1.29          |
| (1,321) | 1:A:86:VAL:HA  | 1:A:87:VAL:HG13 | 9        | 1.29          |
| (1,241) | 1:A:33:GLU:HB3 | 1:A:38:VAL:HA   | 8        | 1.29          |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG11 | 17       | 1.27          |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG12 | 17       | 1.27          |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG13 | 17       | 1.27          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 13       | 1.27          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 6        | 1.27          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 14       | 1.25          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 17       | 1.24          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 18       | 1.24          |
| (1,241) | 1:A:33:GLU:HB3 | 1:A:38:VAL:HA   | 14       | 1.24          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 8        | 1.23          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 15       | 1.23          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 1        | 1.22          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 11       | 1.22          |
| (1,250) | 1:A:75:ALA:HA  | 1:A:79:GLY:HA3  | 3        | 1.21          |
| (1,184) | 1:A:32:SER:HB2 | 1:A:80:TRP:HZ2  | 4        | 1.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 5        | 1.2           |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 10       | 1.2           |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 12       | 1.2           |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 13       | 1.2           |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 16       | 1.2           |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 20       | 1.2           |
| (1,184) | 1:A:32:SER:HB2  | 1:A:80:TRP:HZ2  | 1        | 1.2           |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG11 | 3        | 1.19          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG12 | 3        | 1.19          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG13 | 3        | 1.19          |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 2        | 1.18          |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 4        | 1.18          |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 19       | 1.18          |
| (1,759) | 1:A:32:SER:HB2  | 1:A:39:LEU:H    | 13       | 1.17          |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 7        | 1.17          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 7        | 1.15          |
| (1,250) | 1:A:75:ALA:HA   | 1:A:79:GLY:HA3  | 9        | 1.14          |
| (1,759) | 1:A:32:SER:HB2  | 1:A:39:LEU:H    | 11       | 1.13          |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB   | 18       | 1.1           |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG11 | 17       | 1.08          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG12 | 17       | 1.08          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG13 | 17       | 1.08          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG11 | 17       | 1.08          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG12 | 17       | 1.08          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG13 | 17       | 1.08          |
| (1,184) | 1:A:32:SER:HB2  | 1:A:80:TRP:HZ2  | 11       | 1.08          |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB   | 6        | 1.07          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 8        | 1.06          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 5        | 1.06          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 17       | 1.05          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 17       | 1.05          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 17       | 1.05          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 17       | 1.05          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 17       | 1.05          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 17       | 1.05          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 17       | 1.05          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 17       | 1.05          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 17       | 1.05          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG11 | 2        | 1.05          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG12 | 2        | 1.05          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG13 | 2        | 1.05          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG11 | 2        | 1.05          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG12 | 2        | 1.05          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG13 | 2        | 1.05          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG11 | 4        | 1.05          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG12 | 4        | 1.05          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG13 | 4        | 1.05          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG11 | 4        | 1.05          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG12 | 4        | 1.05          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG13 | 4        | 1.05          |
| (1,335) | 1:A:54:ARG:HB3 | 1:A:86:VAL:HB   | 14       | 1.04          |
| (1,241) | 1:A:33:GLU:HB3 | 1:A:38:VAL:HA   | 10       | 1.04          |
| (1,644) | 1:A:31:PRO:HA  | 1:A:32:SER:HB3  | 4        | 1.03          |
| (1,241) | 1:A:33:GLU:HB3 | 1:A:38:VAL:HA   | 15       | 1.03          |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG11 | 1        | 1.02          |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG12 | 1        | 1.02          |
| (1,662) | 1:A:21:GLU:HG2 | 1:A:87:VAL:HG13 | 1        | 1.02          |
| (1,644) | 1:A:31:PRO:HA  | 1:A:32:SER:HB3  | 11       | 1.01          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG11 | 10       | 1.01          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG12 | 10       | 1.01          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG13 | 10       | 1.01          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG11 | 10       | 1.01          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG12 | 10       | 1.01          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG13 | 10       | 1.01          |
| (1,184) | 1:A:32:SER:HB2 | 1:A:80:TRP:HZ2  | 13       | 1.01          |
| (1,644) | 1:A:31:PRO:HA  | 1:A:32:SER:HB3  | 1        | 1.0           |
| (1,644) | 1:A:31:PRO:HA  | 1:A:32:SER:HB3  | 13       | 1.0           |
| (1,711) | 1:A:68:LEU:HG  | 1:A:73:LEU:HG   | 7        | 0.99          |
| (1,529) | 1:A:55:TYR:HA  | 1:A:83:LEU:HG   | 7        | 0.99          |
| (1,656) | 1:A:54:ARG:HB3 | 1:A:85:TYR:HB2  | 6        | 0.98          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG11 | 3        | 0.98          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG12 | 3        | 0.98          |
| (1,501) | 1:A:85:TYR:HD1 | 1:A:87:VAL:HG13 | 3        | 0.98          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG11 | 3        | 0.98          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG12 | 3        | 0.98          |
| (1,501) | 1:A:85:TYR:HD2 | 1:A:87:VAL:HG13 | 3        | 0.98          |
| (1,464) | 1:A:15:GLU:H   | 1:A:36:GLY:HA3  | 18       | 0.98          |
| (1,656) | 1:A:54:ARG:HB3 | 1:A:85:TYR:HB2  | 18       | 0.97          |
| (1,279) | 1:A:47:PHE:HD1 | 1:A:87:VAL:HG11 | 10       | 0.97          |
| (1,279) | 1:A:47:PHE:HD1 | 1:A:87:VAL:HG12 | 10       | 0.97          |
| (1,279) | 1:A:47:PHE:HD1 | 1:A:87:VAL:HG13 | 10       | 0.97          |
| (1,279) | 1:A:47:PHE:HD2 | 1:A:87:VAL:HG11 | 10       | 0.97          |
| (1,279) | 1:A:47:PHE:HD2 | 1:A:87:VAL:HG12 | 10       | 0.97          |
| (1,279) | 1:A:47:PHE:HD2 | 1:A:87:VAL:HG13 | 10       | 0.97          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 6        | 0.97          |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2  | 14       | 0.96          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG11 | 1        | 0.96          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG12 | 1        | 0.96          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG13 | 1        | 0.96          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG11 | 1        | 0.96          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG12 | 1        | 0.96          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG13 | 1        | 0.96          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG11 | 13       | 0.95          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG12 | 13       | 0.95          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG13 | 13       | 0.95          |
| (1,627) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HA   | 9        | 0.94          |
| (1,529) | 1:A:55:TYR:HA   | 1:A:83:LEU:HG   | 5        | 0.94          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG11 | 9        | 0.94          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG12 | 9        | 0.94          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG13 | 9        | 0.94          |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG11 | 4        | 0.94          |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG12 | 4        | 0.94          |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG13 | 4        | 0.94          |
| (1,759) | 1:A:32:SER:HB2  | 1:A:39:LEU:H    | 1        | 0.93          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 17       | 0.93          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG11 | 1        | 0.93          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG12 | 1        | 0.93          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG13 | 1        | 0.93          |
| (1,464) | 1:A:15:GLU:H    | 1:A:36:GLY:HA3  | 15       | 0.93          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG11 | 4        | 0.92          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG12 | 4        | 0.92          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG13 | 4        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG11 | 2        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG12 | 2        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG13 | 2        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG11 | 3        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG12 | 3        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG13 | 3        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG11 | 4        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG12 | 4        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG13 | 4        | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG11 | 10       | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG12 | 10       | 0.92          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG13 | 10       | 0.92          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 10       | 0.91          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 10       | 0.91          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 10       | 0.91          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 10       | 0.91          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 10       | 0.91          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 10       | 0.91          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 10       | 0.91          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 10       | 0.91          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 10       | 0.91          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG11 | 17       | 0.91          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG12 | 17       | 0.91          |
| (1,488) | 1:A:87:VAL:H    | 1:A:87:VAL:HG13 | 17       | 0.91          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG11 | 4        | 0.91          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG12 | 4        | 0.91          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG13 | 4        | 0.91          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG11 | 4        | 0.91          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG12 | 4        | 0.91          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG13 | 4        | 0.91          |
| (1,890) | 1:A:53:LEU:H    | 1:A:88:ASN:HB2  | 1        | 0.9           |
| (1,890) | 1:A:53:LEU:H    | 1:A:88:ASN:HB3  | 1        | 0.9           |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 8        | 0.9           |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG11 | 17       | 0.89          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG12 | 17       | 0.89          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG13 | 17       | 0.89          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG11 | 17       | 0.89          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG12 | 17       | 0.89          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG13 | 17       | 0.89          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG11 | 11       | 0.89          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG12 | 11       | 0.89          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG13 | 11       | 0.89          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG11 | 3        | 0.89          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG12 | 3        | 0.89          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG13 | 3        | 0.89          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG11 | 3        | 0.89          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG12 | 3        | 0.89          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG13 | 3        | 0.89          |
| (1,890) | 1:A:53:LEU:H    | 1:A:88:ASN:HB2  | 9        | 0.88          |
| (1,890) | 1:A:53:LEU:H    | 1:A:88:ASN:HB3  | 9        | 0.88          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 9        | 0.88          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG11 | 1        | 0.88          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG12 | 1        | 0.88          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG13 | 1        | 0.88          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG11 | 1        | 0.88          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG12 | 1        | 0.88          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG13 | 1        | 0.88          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 18       | 0.88          |
| (1,759) | 1:A:32:SER:HB2  | 1:A:39:LEU:H    | 4        | 0.87          |
| (1,108) | 1:A:6:HIS:H     | 1:A:6:HIS:HD2   | 8        | 0.87          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 15       | 0.86          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 3        | 0.86          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 19       | 0.86          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 20       | 0.84          |
| (1,529) | 1:A:55:TYR:HA   | 1:A:83:LEU:HG   | 13       | 0.84          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 1        | 0.84          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 3        | 0.83          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 1        | 0.82          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 1        | 0.82          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 1        | 0.82          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 1        | 0.82          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 1        | 0.82          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 1        | 0.82          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 1        | 0.82          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 1        | 0.82          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 1        | 0.82          |
| (1,529) | 1:A:55:TYR:HA   | 1:A:83:LEU:HG   | 1        | 0.82          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG11 | 1        | 0.82          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG12 | 1        | 0.82          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG13 | 1        | 0.82          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG11 | 2        | 0.82          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG12 | 2        | 0.82          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG13 | 2        | 0.82          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG11 | 2        | 0.82          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG12 | 2        | 0.82          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG13 | 2        | 0.82          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 5        | 0.8           |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 5        | 0.8           |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 5        | 0.8           |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 2        | 0.8           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 2        | 0.8           |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 2        | 0.8           |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 2        | 0.8           |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 2        | 0.8           |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 2        | 0.8           |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 2        | 0.8           |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 2        | 0.8           |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 2        | 0.8           |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 2        | 0.8           |
| (1,632) | 1:A:54:ARG:HG3  | 1:A:65:GLY:HA2  | 6        | 0.8           |
| (1,632) | 1:A:54:ARG:HG3  | 1:A:65:GLY:HA3  | 6        | 0.8           |
| (1,529) | 1:A:55:TYR:HA   | 1:A:83:LEU:HG   | 14       | 0.8           |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 4        | 0.79          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 4        | 0.79          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 4        | 0.79          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 4        | 0.79          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 4        | 0.79          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 4        | 0.79          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 4        | 0.79          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 4        | 0.79          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 4        | 0.79          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG11 | 9        | 0.79          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG12 | 9        | 0.79          |
| (1,501) | 1:A:85:TYR:HD1  | 1:A:87:VAL:HG13 | 9        | 0.79          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG11 | 9        | 0.79          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG12 | 9        | 0.79          |
| (1,501) | 1:A:85:TYR:HD2  | 1:A:87:VAL:HG13 | 9        | 0.79          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG11 | 4        | 0.79          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG12 | 4        | 0.79          |
| (1,292) | 1:A:32:SER:HB2  | 1:A:38:VAL:HG13 | 4        | 0.79          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 13       | 0.78          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 14       | 0.78          |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG11 | 2        | 0.78          |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG12 | 2        | 0.78          |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG13 | 2        | 0.78          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 2        | 0.78          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 16       | 0.76          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 1        | 0.76          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG11 | 2        | 0.75          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG12 | 2        | 0.75          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG13 | 2        | 0.75          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 5        | 0.75          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 17       | 0.75          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 17       | 0.75          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 17       | 0.75          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG11 | 13       | 0.74          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG12 | 13       | 0.74          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG13 | 13       | 0.74          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG21 | 13       | 0.74          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG22 | 13       | 0.74          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG23 | 13       | 0.74          |
| (1,749) | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 7        | 0.74          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 9        | 0.74          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 9        | 0.74          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 9        | 0.74          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 9        | 0.74          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 9        | 0.74          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 9        | 0.74          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 9        | 0.74          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 9        | 0.74          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 9        | 0.74          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 9        | 0.74          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 13       | 0.74          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 2        | 0.73          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 4        | 0.72          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 4        | 0.72          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 4        | 0.72          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 19       | 0.72          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 4        | 0.72          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 10       | 0.72          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 19       | 0.71          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 16       | 0.71          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 16       | 0.71          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 5        | 0.7           |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 1        | 0.7           |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG11 | 9        | 0.7           |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG12 | 9        | 0.7           |
| (1,309) | 1:A:21:GLU:HB3  | 1:A:87:VAL:HG13 | 9        | 0.7           |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 13       | 0.69          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 13       | 0.69          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 13       | 0.69          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 15       | 0.69          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 15       | 0.69          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 15       | 0.69          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 13       | 0.68          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 7        | 0.68          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 19       | 0.67          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 13       | 0.67          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 13       | 0.67          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 20       | 0.66          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB1  | 13       | 0.66          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB2  | 13       | 0.66          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB3  | 13       | 0.66          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB1  | 13       | 0.66          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB2  | 13       | 0.66          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB3  | 13       | 0.66          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB1  | 13       | 0.66          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB2  | 13       | 0.66          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB3  | 13       | 0.66          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 8        | 0.66          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 14       | 0.66          |
| (1,626) | 1:A:13:MET:HG2  | 1:A:14:SER:HB2  | 10       | 0.66          |
| (1,626) | 1:A:13:MET:HG2  | 1:A:14:SER:HB3  | 10       | 0.66          |
| (1,626) | 1:A:13:MET:HG3  | 1:A:14:SER:HB2  | 10       | 0.66          |
| (1,626) | 1:A:13:MET:HG3  | 1:A:14:SER:HB3  | 10       | 0.66          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 6        | 0.66          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 6        | 0.66          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 6        | 0.66          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 3        | 0.65          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 4        | 0.64          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 4        | 0.64          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 4        | 0.64          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 9        | 0.64          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 9        | 0.64          |
| (1,673) | 1:A:61:GLN:HB2  | 1:A:62:CYS:HA   | 6        | 0.63          |
| (1,673) | 1:A:61:GLN:HB3  | 1:A:62:CYS:HA   | 6        | 0.63          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 10       | 0.63          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 10       | 0.63          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 10       | 0.63          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 13       | 0.63          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 13       | 0.63          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 13       | 0.63          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 13       | 0.63          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 13       | 0.63          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 13       | 0.63          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 17       | 0.63          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 17       | 0.63          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 17       | 0.63          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 17       | 0.63          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 17       | 0.63          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 17       | 0.63          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 8        | 0.63          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 8        | 0.63          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 4        | 0.62          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 5        | 0.62          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 12       | 0.62          |
| (1,627) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HA   | 4        | 0.62          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 4        | 0.62          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 4        | 0.62          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 4        | 0.62          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB1  | 10       | 0.61          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB2  | 10       | 0.61          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB3  | 10       | 0.61          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB1  | 10       | 0.61          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB2  | 10       | 0.61          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB3  | 10       | 0.61          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB1  | 10       | 0.61          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB2  | 10       | 0.61          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB3  | 10       | 0.61          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 8        | 0.61          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 14       | 0.61          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 1        | 0.61          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 6        | 0.61          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 11       | 0.61          |
| (1,626) | 1:A:13:MET:HG2  | 1:A:14:SER:HB2  | 18       | 0.61          |
| (1,626) | 1:A:13:MET:HG2  | 1:A:14:SER:HB3  | 18       | 0.61          |
| (1,626) | 1:A:13:MET:HG3  | 1:A:14:SER:HB2  | 18       | 0.61          |
| (1,626) | 1:A:13:MET:HG3  | 1:A:14:SER:HB3  | 18       | 0.61          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 15       | 0.6           |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 19       | 0.59          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 19       | 0.59          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 19       | 0.59          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 19       | 0.59          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 17       | 0.59          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 15       | 0.59          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 18       | 0.59          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 4        | 0.59          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 12       | 0.59          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 12       | 0.59          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 12       | 0.59          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 12       | 0.59          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 12       | 0.59          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 12       | 0.59          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 7        | 0.59          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 7        | 0.59          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 7        | 0.59          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 7        | 0.58          |
| (1,627) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HA   | 2        | 0.58          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 2        | 0.58          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 3        | 0.57          |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 4        | 0.56          |
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 4        | 0.56          |
| (1,749) | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 17       | 0.56          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB1  | 16       | 0.56          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB2  | 16       | 0.56          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB3  | 16       | 0.56          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB1  | 16       | 0.56          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB2  | 16       | 0.56          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB3  | 16       | 0.56          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB1  | 16       | 0.56          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB2  | 16       | 0.56          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB3  | 16       | 0.56          |
| (1,663) | 1:A:45:ALA:HB1  | 1:A:46:GLN:HG2  | 3        | 0.56          |
| (1,663) | 1:A:45:ALA:HB2  | 1:A:46:GLN:HG2  | 3        | 0.56          |
| (1,663) | 1:A:45:ALA:HB3  | 1:A:46:GLN:HG2  | 3        | 0.56          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 7        | 0.56          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 10       | 0.56          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 3        | 0.56          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 3        | 0.56          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 3        | 0.56          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG11 | 9        | 0.56          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG12 | 9        | 0.56          |
| (1,279) | 1:A:47:PHE:HD1  | 1:A:87:VAL:HG13 | 9        | 0.56          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG11 | 9        | 0.56          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG12 | 9        | 0.56          |
| (1,279) | 1:A:47:PHE:HD2  | 1:A:87:VAL:HG13 | 9        | 0.56          |
| (1,108) | 1:A:6:HIS:H     | 1:A:6:HIS:HD2   | 12       | 0.56          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB1  | 18       | 0.55          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB2  | 18       | 0.55          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB3  | 18       | 0.55          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,723)  | 1:A:37:THR:HG22 | 1:A:75:ALA:HB1  | 18       | 0.55          |
| (1,723)  | 1:A:37:THR:HG22 | 1:A:75:ALA:HB2  | 18       | 0.55          |
| (1,723)  | 1:A:37:THR:HG22 | 1:A:75:ALA:HB3  | 18       | 0.55          |
| (1,723)  | 1:A:37:THR:HG23 | 1:A:75:ALA:HB1  | 18       | 0.55          |
| (1,723)  | 1:A:37:THR:HG23 | 1:A:75:ALA:HB2  | 18       | 0.55          |
| (1,723)  | 1:A:37:THR:HG23 | 1:A:75:ALA:HB3  | 18       | 0.55          |
| (1,636)  | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 20       | 0.55          |
| (1,492)  | 1:A:50:ALA:HB1  | 1:A:52:GLY:H    | 18       | 0.55          |
| (1,492)  | 1:A:50:ALA:HB2  | 1:A:52:GLY:H    | 18       | 0.55          |
| (1,492)  | 1:A:50:ALA:HB3  | 1:A:52:GLY:H    | 18       | 0.55          |
| (1,300)  | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 11       | 0.55          |
| (1,300)  | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 11       | 0.55          |
| (1,300)  | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 11       | 0.55          |
| (1,300)  | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 11       | 0.55          |
| (1,300)  | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 11       | 0.55          |
| (1,300)  | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 11       | 0.55          |
| (1,108)  | 1:A:6:HIS:H     | 1:A:6:HIS:HD2   | 16       | 0.55          |
| (1,1018) | 1:A:84:VAL:HG11 | 1:A:85:TYR:HB3  | 13       | 0.55          |
| (1,1018) | 1:A:84:VAL:HG12 | 1:A:85:TYR:HB3  | 13       | 0.55          |
| (1,1018) | 1:A:84:VAL:HG13 | 1:A:85:TYR:HB3  | 13       | 0.55          |
| (1,1018) | 1:A:84:VAL:HG21 | 1:A:85:TYR:HB3  | 13       | 0.55          |
| (1,1018) | 1:A:84:VAL:HG22 | 1:A:85:TYR:HB3  | 13       | 0.55          |
| (1,1018) | 1:A:84:VAL:HG23 | 1:A:85:TYR:HB3  | 13       | 0.55          |
| (1,723)  | 1:A:37:THR:HG21 | 1:A:75:ALA:HB1  | 1        | 0.54          |
| (1,723)  | 1:A:37:THR:HG21 | 1:A:75:ALA:HB2  | 1        | 0.54          |
| (1,723)  | 1:A:37:THR:HG21 | 1:A:75:ALA:HB3  | 1        | 0.54          |
| (1,723)  | 1:A:37:THR:HG22 | 1:A:75:ALA:HB1  | 1        | 0.54          |
| (1,723)  | 1:A:37:THR:HG22 | 1:A:75:ALA:HB2  | 1        | 0.54          |
| (1,723)  | 1:A:37:THR:HG22 | 1:A:75:ALA:HB3  | 1        | 0.54          |
| (1,723)  | 1:A:37:THR:HG23 | 1:A:75:ALA:HB1  | 1        | 0.54          |
| (1,723)  | 1:A:37:THR:HG23 | 1:A:75:ALA:HB2  | 1        | 0.54          |
| (1,723)  | 1:A:37:THR:HG23 | 1:A:75:ALA:HB3  | 1        | 0.54          |
| (1,526)  | 1:A:29:GLU:HA   | 1:A:30:ILE:HG13 | 10       | 0.54          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 1        | 0.54          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 1        | 0.54          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 1        | 0.54          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 2        | 0.54          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 2        | 0.54          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 2        | 0.54          |
| (1,300)  | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 7        | 0.54          |
| (1,300)  | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 7        | 0.54          |
| (1,300)  | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 7        | 0.54          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 7        | 0.54          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 7        | 0.54          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 7        | 0.54          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 18       | 0.54          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 18       | 0.54          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 11       | 0.53          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 11       | 0.53          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 11       | 0.53          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 6        | 0.53          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 15       | 0.53          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 7        | 0.53          |
| (1,627) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HA   | 18       | 0.53          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 13       | 0.53          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 15       | 0.53          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 15       | 0.53          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 17       | 0.53          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 17       | 0.53          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG11 | 17       | 0.52          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG12 | 17       | 0.52          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG13 | 17       | 0.52          |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB   | 7        | 0.52          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 20       | 0.52          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 20       | 0.52          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 14       | 0.51          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 14       | 0.51          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 14       | 0.51          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 14       | 0.51          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 14       | 0.51          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 14       | 0.51          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 14       | 0.51          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 14       | 0.51          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 14       | 0.51          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB1  | 17       | 0.51          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB2  | 17       | 0.51          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB3  | 17       | 0.51          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB1  | 17       | 0.51          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB2  | 17       | 0.51          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB3  | 17       | 0.51          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB1  | 17       | 0.51          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB2  | 17       | 0.51          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB3  | 17       | 0.51          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 12       | 0.51          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB1  | 16       | 0.51          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB2  | 16       | 0.51          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB3  | 16       | 0.51          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 9        | 0.5           |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 10       | 0.5           |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 1        | 0.5           |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 5        | 0.5           |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 5        | 0.5           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 6        | 0.49          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 6        | 0.49          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 6        | 0.49          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 6        | 0.49          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 6        | 0.49          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 6        | 0.49          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 6        | 0.49          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 6        | 0.49          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 6        | 0.49          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 1        | 0.49          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 13       | 0.49          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 10       | 0.49          |
| (1,503) | 1:A:75:ALA:HB1  | 1:A:80:TRP:HE3  | 15       | 0.49          |
| (1,503) | 1:A:75:ALA:HB2  | 1:A:80:TRP:HE3  | 15       | 0.49          |
| (1,503) | 1:A:75:ALA:HB3  | 1:A:80:TRP:HE3  | 15       | 0.49          |
| (1,303) | 1:A:28:ILE:HG21 | 1:A:46:GLN:HG3  | 12       | 0.49          |
| (1,303) | 1:A:28:ILE:HG22 | 1:A:46:GLN:HG3  | 12       | 0.49          |
| (1,303) | 1:A:28:ILE:HG23 | 1:A:46:GLN:HG3  | 12       | 0.49          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 5        | 0.48          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 4        | 0.48          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 16       | 0.48          |
| (1,691) | 1:A:40:LEU:HB2  | 1:A:40:LEU:HG   | 7        | 0.48          |
| (1,691) | 1:A:40:LEU:HB2  | 1:A:40:LEU:HG   | 11       | 0.48          |
| (1,691) | 1:A:40:LEU:HB2  | 1:A:40:LEU:HG   | 13       | 0.48          |
| (1,691) | 1:A:40:LEU:HB2  | 1:A:40:LEU:HG   | 16       | 0.48          |
| (1,691) | 1:A:40:LEU:HB2  | 1:A:40:LEU:HG   | 18       | 0.48          |
| (1,691) | 1:A:40:LEU:HB2  | 1:A:40:LEU:HG   | 20       | 0.48          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG11 | 9        | 0.48          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG12 | 9        | 0.48          |
| (1,662) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HG13 | 9        | 0.48          |
| (1,492) | 1:A:50:ALA:HB1  | 1:A:52:GLY:H    | 20       | 0.48          |
| (1,492) | 1:A:50:ALA:HB2  | 1:A:52:GLY:H    | 20       | 0.48          |
| (1,492) | 1:A:50:ALA:HB3  | 1:A:52:GLY:H    | 20       | 0.48          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 5        | 0.48          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 5        | 0.48          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 5        | 0.48          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB1  | 5        | 0.47          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB2  | 5        | 0.47          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB3  | 5        | 0.47          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB1  | 5        | 0.47          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB2  | 5        | 0.47          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB3  | 5        | 0.47          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB1  | 5        | 0.47          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB2  | 5        | 0.47          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB3  | 5        | 0.47          |
| (1,492) | 1:A:50:ALA:HB1  | 1:A:52:GLY:H    | 3        | 0.47          |
| (1,492) | 1:A:50:ALA:HB2  | 1:A:52:GLY:H    | 3        | 0.47          |
| (1,492) | 1:A:50:ALA:HB3  | 1:A:52:GLY:H    | 3        | 0.47          |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB   | 8        | 0.47          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 10       | 0.47          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 10       | 0.47          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 10       | 0.47          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 20       | 0.47          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 20       | 0.47          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 17       | 0.46          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 17       | 0.46          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 17       | 0.46          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 17       | 0.46          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 17       | 0.46          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 17       | 0.46          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 17       | 0.46          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 17       | 0.46          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 17       | 0.46          |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2  | 1        | 0.46          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 14       | 0.46          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 15       | 0.46          |
| (1,627) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HA   | 1        | 0.46          |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 7        | 0.45          |
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 7        | 0.45          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 16       | 0.45          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 20       | 0.45          |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2  | 7        | 0.45          |
| (1,632) | 1:A:54:ARG:HG3  | 1:A:65:GLY:HA2  | 14       | 0.45          |
| (1,632) | 1:A:54:ARG:HG3  | 1:A:65:GLY:HA3  | 14       | 0.45          |
| (1,503) | 1:A:75:ALA:HB1  | 1:A:80:TRP:HE3  | 7        | 0.45          |
| (1,503) | 1:A:75:ALA:HB2  | 1:A:80:TRP:HE3  | 7        | 0.45          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,503) | 1:A:75:ALA:HB3  | 1:A:80:TRP:HE3  | 7        | 0.45          |
| (1,303) | 1:A:28:ILE:HG21 | 1:A:46:GLN:HG3  | 13       | 0.45          |
| (1,303) | 1:A:28:ILE:HG22 | 1:A:46:GLN:HG3  | 13       | 0.45          |
| (1,303) | 1:A:28:ILE:HG23 | 1:A:46:GLN:HG3  | 13       | 0.45          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 2        | 0.45          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 2        | 0.45          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 2        | 0.45          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 2        | 0.45          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 3        | 0.45          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 3        | 0.45          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 16       | 0.45          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 16       | 0.45          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 7        | 0.44          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 19       | 0.44          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 19       | 0.44          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 12       | 0.44          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 12       | 0.44          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 18       | 0.43          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 18       | 0.43          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 18       | 0.43          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 18       | 0.43          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 18       | 0.43          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 18       | 0.43          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 18       | 0.43          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 18       | 0.43          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 18       | 0.43          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 15       | 0.43          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 18       | 0.43          |
| (1,503) | 1:A:75:ALA:HB1  | 1:A:80:TRP:HE3  | 3        | 0.43          |
| (1,503) | 1:A:75:ALA:HB2  | 1:A:80:TRP:HE3  | 3        | 0.43          |
| (1,503) | 1:A:75:ALA:HB3  | 1:A:80:TRP:HE3  | 3        | 0.43          |
| (1,314) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 11       | 0.43          |
| (1,314) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 11       | 0.43          |
| (1,314) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 11       | 0.43          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 8        | 0.43          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 8        | 0.43          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 3        | 0.42          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 11       | 0.42          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 6        | 0.42          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 17       | 0.42          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 10       | 0.42          |
| (1,636) | 1:A:52:GLY:HA3  | 1:A:68:LEU:HG   | 17       | 0.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,503) | 1:A:75:ALA:HB1  | 1:A:80:TRP:HE3  | 5        | 0.42          |
| (1,503) | 1:A:75:ALA:HB2  | 1:A:80:TRP:HE3  | 5        | 0.42          |
| (1,503) | 1:A:75:ALA:HB3  | 1:A:80:TRP:HE3  | 5        | 0.42          |
| (1,503) | 1:A:75:ALA:HB1  | 1:A:80:TRP:HE3  | 6        | 0.42          |
| (1,503) | 1:A:75:ALA:HB2  | 1:A:80:TRP:HE3  | 6        | 0.42          |
| (1,503) | 1:A:75:ALA:HB3  | 1:A:80:TRP:HE3  | 6        | 0.42          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 4        | 0.42          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 4        | 0.42          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 16       | 0.42          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 16       | 0.42          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 1        | 0.42          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 1        | 0.42          |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 1        | 0.41          |
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 1        | 0.41          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 10       | 0.41          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 10       | 0.41          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 10       | 0.41          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 10       | 0.41          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 10       | 0.41          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 10       | 0.41          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 10       | 0.41          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 10       | 0.41          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 10       | 0.41          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB1  | 11       | 0.41          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB2  | 11       | 0.41          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB3  | 11       | 0.41          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB1  | 11       | 0.41          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB2  | 11       | 0.41          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB3  | 11       | 0.41          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB1  | 11       | 0.41          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB2  | 11       | 0.41          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB3  | 11       | 0.41          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 14       | 0.41          |
| (1,314) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 2        | 0.41          |
| (1,314) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 2        | 0.41          |
| (1,314) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 2        | 0.41          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 9        | 0.41          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 9        | 0.41          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 9        | 0.41          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 4        | 0.41          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 4        | 0.41          |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 14       | 0.4           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 14       | 0.4           |
| (1,503) | 1:A:75:ALA:HB1  | 1:A:80:TRP:HE3  | 9        | 0.4           |
| (1,503) | 1:A:75:ALA:HB2  | 1:A:80:TRP:HE3  | 9        | 0.4           |
| (1,503) | 1:A:75:ALA:HB3  | 1:A:80:TRP:HE3  | 9        | 0.4           |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 12       | 0.4           |
| (1,314) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 12       | 0.4           |
| (1,314) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 12       | 0.4           |
| (1,314) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 12       | 0.4           |
| (1,314) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 13       | 0.4           |
| (1,314) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 13       | 0.4           |
| (1,314) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 13       | 0.4           |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 12       | 0.4           |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 12       | 0.4           |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 12       | 0.4           |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 19       | 0.4           |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 19       | 0.4           |
| (1,108) | 1:A:6:HIS:H     | 1:A:6:HIS:HD2   | 20       | 0.4           |
| (1,874) | 1:A:40:LEU:HD11 | 1:A:41:SER:HA   | 13       | 0.39          |
| (1,874) | 1:A:40:LEU:HD12 | 1:A:41:SER:HA   | 13       | 0.39          |
| (1,874) | 1:A:40:LEU:HD13 | 1:A:41:SER:HA   | 13       | 0.39          |
| (1,874) | 1:A:40:LEU:HD21 | 1:A:41:SER:HA   | 13       | 0.39          |
| (1,874) | 1:A:40:LEU:HD22 | 1:A:41:SER:HA   | 13       | 0.39          |
| (1,874) | 1:A:40:LEU:HD23 | 1:A:41:SER:HA   | 13       | 0.39          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB1  | 19       | 0.39          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB2  | 19       | 0.39          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB3  | 19       | 0.39          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB1  | 19       | 0.39          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB2  | 19       | 0.39          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB3  | 19       | 0.39          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB1  | 19       | 0.39          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB2  | 19       | 0.39          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB3  | 19       | 0.39          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 10       | 0.39          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 6        | 0.39          |
| (1,492) | 1:A:50:ALA:HB1  | 1:A:52:GLY:H    | 10       | 0.39          |
| (1,492) | 1:A:50:ALA:HB2  | 1:A:52:GLY:H    | 10       | 0.39          |
| (1,492) | 1:A:50:ALA:HB3  | 1:A:52:GLY:H    | 10       | 0.39          |
| (1,314) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 20       | 0.39          |
| (1,314) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 20       | 0.39          |
| (1,314) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 20       | 0.39          |
| (1,874) | 1:A:40:LEU:HD11 | 1:A:41:SER:HA   | 16       | 0.38          |
| (1,874) | 1:A:40:LEU:HD12 | 1:A:41:SER:HA   | 16       | 0.38          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,874) | 1:A:40:LEU:HD13 | 1:A:41:SER:HA   | 16       | 0.38          |
| (1,874) | 1:A:40:LEU:HD21 | 1:A:41:SER:HA   | 16       | 0.38          |
| (1,874) | 1:A:40:LEU:HD22 | 1:A:41:SER:HA   | 16       | 0.38          |
| (1,874) | 1:A:40:LEU:HD23 | 1:A:41:SER:HA   | 16       | 0.38          |
| (1,874) | 1:A:40:LEU:HD11 | 1:A:41:SER:HA   | 20       | 0.38          |
| (1,874) | 1:A:40:LEU:HD12 | 1:A:41:SER:HA   | 20       | 0.38          |
| (1,874) | 1:A:40:LEU:HD13 | 1:A:41:SER:HA   | 20       | 0.38          |
| (1,874) | 1:A:40:LEU:HD21 | 1:A:41:SER:HA   | 20       | 0.38          |
| (1,874) | 1:A:40:LEU:HD22 | 1:A:41:SER:HA   | 20       | 0.38          |
| (1,874) | 1:A:40:LEU:HD23 | 1:A:41:SER:HA   | 20       | 0.38          |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 10       | 0.38          |
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 10       | 0.38          |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA   | 10       | 0.38          |
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 10       | 0.38          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG11 | 4        | 0.38          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG12 | 4        | 0.38          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG13 | 4        | 0.38          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 12       | 0.38          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB1  | 2        | 0.38          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB2  | 2        | 0.38          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB3  | 2        | 0.38          |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB   | 1        | 0.38          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 1        | 0.38          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 1        | 0.38          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 1        | 0.38          |
| (1,874) | 1:A:40:LEU:HD11 | 1:A:41:SER:HA   | 11       | 0.37          |
| (1,874) | 1:A:40:LEU:HD12 | 1:A:41:SER:HA   | 11       | 0.37          |
| (1,874) | 1:A:40:LEU:HD13 | 1:A:41:SER:HA   | 11       | 0.37          |
| (1,874) | 1:A:40:LEU:HD21 | 1:A:41:SER:HA   | 11       | 0.37          |
| (1,874) | 1:A:40:LEU:HD22 | 1:A:41:SER:HA   | 11       | 0.37          |
| (1,874) | 1:A:40:LEU:HD23 | 1:A:41:SER:HA   | 11       | 0.37          |
| (1,830) | 1:A:29:GLU:H    | 1:A:29:GLU:HG2  | 19       | 0.37          |
| (1,830) | 1:A:29:GLU:H    | 1:A:29:GLU:HG3  | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 4        | 0.37          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 4        | 0.37          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 4        | 0.37          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 4        | 0.37          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 4        | 0.37          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 4        | 0.37          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 4        | 0.37          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 4        | 0.37          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 4        | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 19       | 0.37          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 19       | 0.37          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB1  | 14       | 0.37          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB2  | 14       | 0.37          |
| (1,723) | 1:A:37:THR:HG21 | 1:A:75:ALA:HB3  | 14       | 0.37          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB1  | 14       | 0.37          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB2  | 14       | 0.37          |
| (1,723) | 1:A:37:THR:HG22 | 1:A:75:ALA:HB3  | 14       | 0.37          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB1  | 14       | 0.37          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB2  | 14       | 0.37          |
| (1,723) | 1:A:37:THR:HG23 | 1:A:75:ALA:HB3  | 14       | 0.37          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 6        | 0.37          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 6        | 0.37          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 6        | 0.37          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 14       | 0.37          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 14       | 0.37          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 14       | 0.37          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 2        | 0.37          |
| (1,663) | 1:A:45:ALA:HB1  | 1:A:46:GLN:HG2  | 12       | 0.37          |
| (1,663) | 1:A:45:ALA:HB2  | 1:A:46:GLN:HG2  | 12       | 0.37          |
| (1,663) | 1:A:45:ALA:HB3  | 1:A:46:GLN:HG2  | 12       | 0.37          |
| (1,653) | 1:A:21:GLU:HB2  | 1:A:47:PHE:HB3  | 11       | 0.37          |
| (1,503) | 1:A:75:ALA:HB1  | 1:A:80:TRP:HE3  | 19       | 0.37          |
| (1,503) | 1:A:75:ALA:HB2  | 1:A:80:TRP:HE3  | 19       | 0.37          |
| (1,503) | 1:A:75:ALA:HB3  | 1:A:80:TRP:HE3  | 19       | 0.37          |
| (1,314) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 4        | 0.37          |
| (1,314) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 4        | 0.37          |
| (1,314) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 4        | 0.37          |
| (1,874) | 1:A:40:LEU:HD11 | 1:A:41:SER:HA   | 7        | 0.36          |
| (1,874) | 1:A:40:LEU:HD12 | 1:A:41:SER:HA   | 7        | 0.36          |
| (1,874) | 1:A:40:LEU:HD13 | 1:A:41:SER:HA   | 7        | 0.36          |
| (1,874) | 1:A:40:LEU:HD21 | 1:A:41:SER:HA   | 7        | 0.36          |
| (1,874) | 1:A:40:LEU:HD22 | 1:A:41:SER:HA   | 7        | 0.36          |
| (1,874) | 1:A:40:LEU:HD23 | 1:A:41:SER:HA   | 7        | 0.36          |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA   | 8        | 0.36          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 8        | 0.36          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 2        | 0.36          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 3        | 0.36          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 3        | 0.36          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 3        | 0.36          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 3        | 0.36          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 3        | 0.36          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 3        | 0.36          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 3        | 0.36          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 3        | 0.36          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 3        | 0.36          |
| (1,693) | 1:A:30:ILE:HB   | 1:A:46:GLN:HG2  | 8        | 0.36          |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2  | 13       | 0.36          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 14       | 0.36          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 6        | 0.36          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 13       | 0.36          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 13       | 0.35          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 13       | 0.35          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 13       | 0.35          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 13       | 0.35          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 13       | 0.35          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 13       | 0.35          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 13       | 0.35          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 13       | 0.35          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 13       | 0.35          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 15       | 0.35          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 15       | 0.35          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 15       | 0.35          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 20       | 0.35          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 20       | 0.35          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 20       | 0.35          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 8        | 0.35          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 12       | 0.35          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 14       | 0.35          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 18       | 0.35          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 3        | 0.35          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 3        | 0.35          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 3        | 0.35          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 3        | 0.35          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 3        | 0.35          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 3        | 0.35          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 7        | 0.35          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 7        | 0.35          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 13       | 0.35          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 13       | 0.35          |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA   | 19       | 0.34          |
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 19       | 0.34          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 15       | 0.34          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 15       | 0.34          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 15       | 0.34          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 15       | 0.34          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 15       | 0.34          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 15       | 0.34          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 15       | 0.34          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 15       | 0.34          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 15       | 0.34          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD11 | 20       | 0.34          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD12 | 20       | 0.34          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD13 | 20       | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 5        | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 5        | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 5        | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 11       | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 11       | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 11       | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 18       | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 18       | 0.34          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 18       | 0.34          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 8        | 0.34          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 3        | 0.34          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 12       | 0.34          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 12       | 0.34          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 12       | 0.34          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 13       | 0.34          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 13       | 0.34          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 13       | 0.34          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 8        | 0.34          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 8        | 0.34          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 8        | 0.34          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 9        | 0.34          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 9        | 0.34          |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA   | 14       | 0.33          |
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 14       | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 1        | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 9        | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 20       | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 20       | 0.33          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 20       | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 20       | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 20       | 0.33          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 20       | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 20       | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 20       | 0.33          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 20       | 0.33          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG11 | 10       | 0.33          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG12 | 10       | 0.33          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG13 | 10       | 0.33          |
| (1,711) | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 18       | 0.33          |
| (1,642) | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3  | 15       | 0.33          |
| (1,642) | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3  | 15       | 0.33          |
| (1,642) | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3  | 15       | 0.33          |
| (1,439) | 1:A:39:LEU:H    | 1:A:39:LEU:HG   | 16       | 0.33          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 17       | 0.33          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 17       | 0.33          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 9        | 0.33          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 9        | 0.33          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 12       | 0.33          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 12       | 0.33          |
| (1,749) | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 19       | 0.32          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 17       | 0.32          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 17       | 0.32          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 17       | 0.32          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 11       | 0.32          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 8        | 0.32          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 17       | 0.32          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 17       | 0.32          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 17       | 0.32          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 6        | 0.32          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 6        | 0.32          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 1        | 0.31          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 1        | 0.31          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 1        | 0.31          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 12       | 0.31          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 16       | 0.31          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 16       | 0.31          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 16       | 0.31          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 16       | 0.31          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 16       | 0.31          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 16       | 0.31          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 16       | 0.31          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 16       | 0.31          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 16       | 0.31          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD11 | 14       | 0.31          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD12 | 14       | 0.31          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD13 | 14       | 0.31          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 18       | 0.31          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 1        | 0.31          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 16       | 0.31          |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 18       | 0.31          |
| (1,790) | 1:A:15:GLU:HB2  | 1:A:36:GLY:HA3  | 16       | 0.3           |
| (1,790) | 1:A:15:GLU:HB3  | 1:A:36:GLY:HA3  | 16       | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 5        | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 8        | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 11       | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 11       | 0.3           |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 11       | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 11       | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 11       | 0.3           |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 11       | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 11       | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 11       | 0.3           |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 11       | 0.3           |
| (1,746) | 1:A:40:LEU:HA   | 1:A:71:GLY:HA3  | 1        | 0.3           |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG11 | 3        | 0.3           |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG12 | 3        | 0.3           |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG13 | 3        | 0.3           |
| (1,642) | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3  | 2        | 0.3           |
| (1,642) | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3  | 2        | 0.3           |
| (1,642) | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3  | 2        | 0.3           |
| (1,642) | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3  | 4        | 0.3           |
| (1,642) | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3  | 4        | 0.3           |
| (1,642) | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3  | 4        | 0.3           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1 | 4        | 0.3           |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1 | 18       | 0.3           |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2 | 18       | 0.3           |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1 | 18       | 0.3           |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2 | 18       | 0.3           |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1 | 18       | 0.3           |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2 | 18       | 0.3           |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3 | 5        | 0.3           |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3 | 5        | 0.3           |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3 | 5        | 0.3           |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1 | 12       | 0.29          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2 | 12       | 0.29          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3 | 12       | 0.29          |
| (1,896) | 1:A:53:LEU:HD11 | 1:A:73:LEU:HB3 | 18       | 0.29          |
| (1,896) | 1:A:53:LEU:HD12 | 1:A:73:LEU:HB3 | 18       | 0.29          |
| (1,896) | 1:A:53:LEU:HD13 | 1:A:73:LEU:HB3 | 18       | 0.29          |
| (1,896) | 1:A:53:LEU:HD21 | 1:A:73:LEU:HB3 | 18       | 0.29          |
| (1,896) | 1:A:53:LEU:HD22 | 1:A:73:LEU:HB3 | 18       | 0.29          |
| (1,896) | 1:A:53:LEU:HD23 | 1:A:73:LEU:HB3 | 18       | 0.29          |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA  | 1        | 0.29          |
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA  | 1        | 0.29          |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA  | 18       | 0.29          |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA  | 18       | 0.29          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3 | 18       | 0.29          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1 | 9        | 0.29          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1 | 18       | 0.29          |
| (1,496) | 1:A:32:SER:HB3  | 1:A:80:TRP:HD1 | 13       | 0.29          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA  | 12       | 0.29          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1 | 18       | 0.29          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2 | 18       | 0.29          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1 | 8        | 0.29          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2 | 8        | 0.29          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG  | 5        | 0.28          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG  | 5        | 0.28          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG  | 5        | 0.28          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG  | 5        | 0.28          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG  | 5        | 0.28          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG  | 5        | 0.28          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG  | 8        | 0.28          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG  | 8        | 0.28          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG  | 8        | 0.28          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG  | 8        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,990)  | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 8        | 0.28          |
| (1,990)  | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 8        | 0.28          |
| (1,896)  | 1:A:53:LEU:HD11 | 1:A:73:LEU:HB3  | 6        | 0.28          |
| (1,896)  | 1:A:53:LEU:HD12 | 1:A:73:LEU:HB3  | 6        | 0.28          |
| (1,896)  | 1:A:53:LEU:HD13 | 1:A:73:LEU:HB3  | 6        | 0.28          |
| (1,896)  | 1:A:53:LEU:HD21 | 1:A:73:LEU:HB3  | 6        | 0.28          |
| (1,896)  | 1:A:53:LEU:HD22 | 1:A:73:LEU:HB3  | 6        | 0.28          |
| (1,896)  | 1:A:53:LEU:HD23 | 1:A:73:LEU:HB3  | 6        | 0.28          |
| (1,896)  | 1:A:53:LEU:HD11 | 1:A:73:LEU:HB3  | 15       | 0.28          |
| (1,896)  | 1:A:53:LEU:HD12 | 1:A:73:LEU:HB3  | 15       | 0.28          |
| (1,896)  | 1:A:53:LEU:HD13 | 1:A:73:LEU:HB3  | 15       | 0.28          |
| (1,896)  | 1:A:53:LEU:HD21 | 1:A:73:LEU:HB3  | 15       | 0.28          |
| (1,896)  | 1:A:53:LEU:HD22 | 1:A:73:LEU:HB3  | 15       | 0.28          |
| (1,896)  | 1:A:53:LEU:HD23 | 1:A:73:LEU:HB3  | 15       | 0.28          |
| (1,746)  | 1:A:40:LEU:HA   | 1:A:71:GLY:HA3  | 9        | 0.28          |
| (1,715)  | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 8        | 0.28          |
| (1,715)  | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 8        | 0.28          |
| (1,715)  | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 8        | 0.28          |
| (1,704)  | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 15       | 0.28          |
| (1,704)  | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 15       | 0.28          |
| (1,693)  | 1:A:30:ILE:HB   | 1:A:46:GLN:HG2  | 13       | 0.28          |
| (1,645)  | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 8        | 0.28          |
| (1,645)  | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 12       | 0.28          |
| (1,641)  | 1:A:43:VAL:HA   | 1:A:45:ALA:HB1  | 11       | 0.28          |
| (1,641)  | 1:A:43:VAL:HA   | 1:A:45:ALA:HB2  | 11       | 0.28          |
| (1,641)  | 1:A:43:VAL:HA   | 1:A:45:ALA:HB3  | 11       | 0.28          |
| (1,589)  | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 20       | 0.28          |
| (1,563)  | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 19       | 0.28          |
| (1,480)  | 1:A:75:ALA:HB1  | 1:A:79:GLY:H    | 2        | 0.28          |
| (1,480)  | 1:A:75:ALA:HB2  | 1:A:79:GLY:H    | 2        | 0.28          |
| (1,480)  | 1:A:75:ALA:HB3  | 1:A:79:GLY:H    | 2        | 0.28          |
| (1,480)  | 1:A:75:ALA:HB1  | 1:A:79:GLY:H    | 11       | 0.28          |
| (1,480)  | 1:A:75:ALA:HB2  | 1:A:79:GLY:H    | 11       | 0.28          |
| (1,480)  | 1:A:75:ALA:HB3  | 1:A:79:GLY:H    | 11       | 0.28          |
| (1,480)  | 1:A:75:ALA:HB1  | 1:A:79:GLY:H    | 13       | 0.28          |
| (1,480)  | 1:A:75:ALA:HB2  | 1:A:79:GLY:H    | 13       | 0.28          |
| (1,480)  | 1:A:75:ALA:HB3  | 1:A:79:GLY:H    | 13       | 0.28          |
| (1,131)  | 1:A:55:TYR:HD1  | 1:A:83:LEU:HG   | 7        | 0.28          |
| (1,131)  | 1:A:55:TYR:HD2  | 1:A:83:LEU:HG   | 7        | 0.28          |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD11 | 20       | 0.28          |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD12 | 20       | 0.28          |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD13 | 20       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD11 | 20       | 0.28          |
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD12 | 20       | 0.28          |
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD13 | 20       | 0.28          |
| (1,990)  | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 12       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 12       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 12       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 12       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 12       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 12       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 18       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 18       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 18       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 18       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 18       | 0.27          |
| (1,990)  | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 18       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD11 | 1:A:73:LEU:HB3  | 14       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD12 | 1:A:73:LEU:HB3  | 14       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD13 | 1:A:73:LEU:HB3  | 14       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD21 | 1:A:73:LEU:HB3  | 14       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD22 | 1:A:73:LEU:HB3  | 14       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD23 | 1:A:73:LEU:HB3  | 14       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD11 | 1:A:73:LEU:HB3  | 17       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD12 | 1:A:73:LEU:HB3  | 17       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD13 | 1:A:73:LEU:HB3  | 17       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD21 | 1:A:73:LEU:HB3  | 17       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD22 | 1:A:73:LEU:HB3  | 17       | 0.27          |
| (1,896)  | 1:A:53:LEU:HD23 | 1:A:73:LEU:HB3  | 17       | 0.27          |
| (1,749)  | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 4        | 0.27          |
| (1,711)  | 1:A:68:LEU:HG   | 1:A:73:LEU:HG   | 6        | 0.27          |
| (1,693)  | 1:A:30:ILE:HB   | 1:A:46:GLN:HG2  | 12       | 0.27          |
| (1,693)  | 1:A:30:ILE:HB   | 1:A:46:GLN:HG2  | 15       | 0.27          |
| (1,642)  | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3  | 14       | 0.27          |
| (1,642)  | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3  | 14       | 0.27          |
| (1,642)  | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3  | 14       | 0.27          |
| (1,642)  | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3  | 16       | 0.27          |
| (1,642)  | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3  | 16       | 0.27          |
| (1,642)  | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3  | 16       | 0.27          |
| (1,641)  | 1:A:43:VAL:HA   | 1:A:45:ALA:HB1  | 3        | 0.27          |
| (1,641)  | 1:A:43:VAL:HA   | 1:A:45:ALA:HB2  | 3        | 0.27          |
| (1,641)  | 1:A:43:VAL:HA   | 1:A:45:ALA:HB3  | 3        | 0.27          |
| (1,625)  | 1:A:21:GLU:HG2  | 1:A:87:VAL:HA   | 10       | 0.27          |
| (1,589)  | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 7        | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,480) | 1:A:75:ALA:HB1  | 1:A:79:GLY:H    | 20       | 0.27          |
| (1,480) | 1:A:75:ALA:HB2  | 1:A:79:GLY:H    | 20       | 0.27          |
| (1,480) | 1:A:75:ALA:HB3  | 1:A:79:GLY:H    | 20       | 0.27          |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB   | 16       | 0.27          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 4        | 0.27          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 4        | 0.27          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 4        | 0.27          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 4        | 0.27          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 4        | 0.27          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 4        | 0.27          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 20       | 0.27          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 20       | 0.27          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 20       | 0.27          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 20       | 0.27          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 20       | 0.27          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 20       | 0.27          |
| (1,131) | 1:A:55:TYR:HD1  | 1:A:83:LEU:HG   | 5        | 0.27          |
| (1,131) | 1:A:55:TYR:HD2  | 1:A:83:LEU:HG   | 5        | 0.27          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 6        | 0.26          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 6        | 0.26          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 6        | 0.26          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 6        | 0.26          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 6        | 0.26          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 6        | 0.26          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 14       | 0.26          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 14       | 0.26          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 14       | 0.26          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 14       | 0.26          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 14       | 0.26          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 14       | 0.26          |
| (1,874) | 1:A:40:LEU:HD11 | 1:A:41:SER:HA   | 18       | 0.26          |
| (1,874) | 1:A:40:LEU:HD12 | 1:A:41:SER:HA   | 18       | 0.26          |
| (1,874) | 1:A:40:LEU:HD13 | 1:A:41:SER:HA   | 18       | 0.26          |
| (1,874) | 1:A:40:LEU:HD21 | 1:A:41:SER:HA   | 18       | 0.26          |
| (1,874) | 1:A:40:LEU:HD22 | 1:A:41:SER:HA   | 18       | 0.26          |
| (1,874) | 1:A:40:LEU:HD23 | 1:A:41:SER:HA   | 18       | 0.26          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG21 | 7        | 0.26          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG22 | 7        | 0.26          |
| (1,753) | 1:A:86:VAL:HG21 | 1:A:87:VAL:HG23 | 7        | 0.26          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG21 | 7        | 0.26          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG22 | 7        | 0.26          |
| (1,753) | 1:A:86:VAL:HG22 | 1:A:87:VAL:HG23 | 7        | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG21 | 7        | 0.26          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG22 | 7        | 0.26          |
| (1,753) | 1:A:86:VAL:HG23 | 1:A:87:VAL:HG23 | 7        | 0.26          |
| (1,749) | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 14       | 0.26          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 16       | 0.26          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 16       | 0.26          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 16       | 0.26          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 19       | 0.26          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 19       | 0.26          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 19       | 0.26          |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 20       | 0.26          |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 20       | 0.26          |
| (1,693) | 1:A:30:ILE:HB   | 1:A:46:GLN:HG2  | 3        | 0.26          |
| (1,672) | 1:A:69:VAL:HG21 | 1:A:70:GLU:HG2  | 7        | 0.26          |
| (1,672) | 1:A:69:VAL:HG21 | 1:A:70:GLU:HG3  | 7        | 0.26          |
| (1,672) | 1:A:69:VAL:HG22 | 1:A:70:GLU:HG2  | 7        | 0.26          |
| (1,672) | 1:A:69:VAL:HG22 | 1:A:70:GLU:HG3  | 7        | 0.26          |
| (1,672) | 1:A:69:VAL:HG23 | 1:A:70:GLU:HG2  | 7        | 0.26          |
| (1,672) | 1:A:69:VAL:HG23 | 1:A:70:GLU:HG3  | 7        | 0.26          |
| (1,642) | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3  | 9        | 0.26          |
| (1,642) | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3  | 9        | 0.26          |
| (1,642) | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3  | 9        | 0.26          |
| (1,642) | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3  | 10       | 0.26          |
| (1,642) | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3  | 10       | 0.26          |
| (1,642) | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3  | 10       | 0.26          |
| (1,625) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HA   | 3        | 0.26          |
| (1,625) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HA   | 17       | 0.26          |
| (1,480) | 1:A:75:ALA:HB1  | 1:A:79:GLY:H    | 4        | 0.26          |
| (1,480) | 1:A:75:ALA:HB2  | 1:A:79:GLY:H    | 4        | 0.26          |
| (1,480) | 1:A:75:ALA:HB3  | 1:A:79:GLY:H    | 4        | 0.26          |
| (1,480) | 1:A:75:ALA:HB1  | 1:A:79:GLY:H    | 12       | 0.26          |
| (1,480) | 1:A:75:ALA:HB2  | 1:A:79:GLY:H    | 12       | 0.26          |
| (1,480) | 1:A:75:ALA:HB3  | 1:A:79:GLY:H    | 12       | 0.26          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 17       | 0.26          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 18       | 0.26          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 18       | 0.26          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 18       | 0.26          |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 16       | 0.26          |
| (1,131) | 1:A:55:TYR:HD1  | 1:A:83:LEU:HG   | 1        | 0.26          |
| (1,131) | 1:A:55:TYR:HD2  | 1:A:83:LEU:HG   | 1        | 0.26          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 3        | 0.25          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 3        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 3        | 0.25          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 3        | 0.25          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 3        | 0.25          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 3        | 0.25          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 17       | 0.25          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 17       | 0.25          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 17       | 0.25          |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 13       | 0.25          |
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 13       | 0.25          |
| (1,746) | 1:A:40:LEU:HA   | 1:A:71:GLY:HA3  | 2        | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 1        | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 1        | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 1        | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 9        | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 9        | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 9        | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 10       | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 10       | 0.25          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 10       | 0.25          |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 2        | 0.25          |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 2        | 0.25          |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 11       | 0.25          |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 11       | 0.25          |
| (1,693) | 1:A:30:ILE:HB   | 1:A:46:GLN:HG2  | 9        | 0.25          |
| (1,672) | 1:A:69:VAL:HG21 | 1:A:70:GLU:HG2  | 17       | 0.25          |
| (1,672) | 1:A:69:VAL:HG21 | 1:A:70:GLU:HG3  | 17       | 0.25          |
| (1,672) | 1:A:69:VAL:HG22 | 1:A:70:GLU:HG2  | 17       | 0.25          |
| (1,672) | 1:A:69:VAL:HG22 | 1:A:70:GLU:HG3  | 17       | 0.25          |
| (1,672) | 1:A:69:VAL:HG23 | 1:A:70:GLU:HG2  | 17       | 0.25          |
| (1,672) | 1:A:69:VAL:HG23 | 1:A:70:GLU:HG3  | 17       | 0.25          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB1  | 14       | 0.25          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB2  | 14       | 0.25          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB3  | 14       | 0.25          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 6        | 0.25          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 13       | 0.25          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB1  | 15       | 0.25          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB2  | 15       | 0.25          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB3  | 15       | 0.25          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 9        | 0.25          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 9        | 0.25          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 9        | 0.25          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 9        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 9        | 0.25          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 9        | 0.25          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 11       | 0.25          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 11       | 0.25          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 11       | 0.25          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 13       | 0.25          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 13       | 0.25          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 13       | 0.25          |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 8        | 0.25          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 1        | 0.25          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 1        | 0.25          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 3        | 0.25          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 3        | 0.25          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 19       | 0.25          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 19       | 0.25          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 11       | 0.25          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 11       | 0.25          |
| (1,131) | 1:A:55:TYR:HD1  | 1:A:83:LEU:HG   | 13       | 0.25          |
| (1,131) | 1:A:55:TYR:HD2  | 1:A:83:LEU:HG   | 13       | 0.25          |
| (1,967) | 1:A:66:VAL:HG11 | 1:A:85:TYR:HA   | 3        | 0.24          |
| (1,967) | 1:A:66:VAL:HG12 | 1:A:85:TYR:HA   | 3        | 0.24          |
| (1,967) | 1:A:66:VAL:HG13 | 1:A:85:TYR:HA   | 3        | 0.24          |
| (1,967) | 1:A:66:VAL:HG21 | 1:A:85:TYR:HA   | 3        | 0.24          |
| (1,967) | 1:A:66:VAL:HG22 | 1:A:85:TYR:HA   | 3        | 0.24          |
| (1,967) | 1:A:66:VAL:HG23 | 1:A:85:TYR:HA   | 3        | 0.24          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 18       | 0.24          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 18       | 0.24          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 18       | 0.24          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 18       | 0.24          |
| (1,790) | 1:A:15:GLU:HB2  | 1:A:36:GLY:HA3  | 3        | 0.24          |
| (1,790) | 1:A:15:GLU:HB3  | 1:A:36:GLY:HA3  | 3        | 0.24          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 7        | 0.24          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 7        | 0.24          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 7        | 0.24          |
| (1,625) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HA   | 9        | 0.24          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 10       | 0.24          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 17       | 0.24          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 13       | 0.24          |
| (1,496) | 1:A:32:SER:HB3  | 1:A:80:TRP:HD1  | 4        | 0.24          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 1        | 0.24          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 15       | 0.24          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 15       | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 15       | 0.24          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 15       | 0.24          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 15       | 0.24          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 15       | 0.24          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 4        | 0.24          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 19       | 0.24          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 19       | 0.24          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 19       | 0.24          |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 2        | 0.24          |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 7        | 0.24          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 11       | 0.24          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 11       | 0.24          |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 1        | 0.24          |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 4        | 0.24          |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 15       | 0.24          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 15       | 0.23          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 15       | 0.23          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 15       | 0.23          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 15       | 0.23          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 15       | 0.23          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 15       | 0.23          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 16       | 0.23          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 16       | 0.23          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 16       | 0.23          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 16       | 0.23          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 16       | 0.23          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 16       | 0.23          |
| (1,893) | 1:A:53:LEU:HD11 | 1:A:54:ARG:H    | 17       | 0.23          |
| (1,893) | 1:A:53:LEU:HD12 | 1:A:54:ARG:H    | 17       | 0.23          |
| (1,893) | 1:A:53:LEU:HD13 | 1:A:54:ARG:H    | 17       | 0.23          |
| (1,893) | 1:A:53:LEU:HD21 | 1:A:54:ARG:H    | 17       | 0.23          |
| (1,893) | 1:A:53:LEU:HD22 | 1:A:54:ARG:H    | 17       | 0.23          |
| (1,893) | 1:A:53:LEU:HD23 | 1:A:54:ARG:H    | 17       | 0.23          |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB1  | 11       | 0.23          |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB2  | 11       | 0.23          |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB3  | 11       | 0.23          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG11 | 1        | 0.23          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG12 | 1        | 0.23          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG13 | 1        | 0.23          |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 9        | 0.23          |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 9        | 0.23          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 6        | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 6        | 0.23          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 6        | 0.23          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 12       | 0.23          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 14       | 0.23          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 2        | 0.23          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 7        | 0.23          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 2        | 0.23          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 2        | 0.23          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 2        | 0.23          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 2        | 0.23          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 2        | 0.23          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 2        | 0.23          |
| (1,241) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 11       | 0.23          |
| (1,163) | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE1  | 9        | 0.23          |
| (1,163) | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE2  | 9        | 0.23          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 5        | 0.23          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 5        | 0.23          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 14       | 0.23          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 14       | 0.23          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 2        | 0.22          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 2        | 0.22          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 2        | 0.22          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 2        | 0.22          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 2        | 0.22          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 2        | 0.22          |
| (1,888) | 1:A:52:GLY:HA3  | 1:A:88:ASN:HB2  | 9        | 0.22          |
| (1,888) | 1:A:52:GLY:HA3  | 1:A:88:ASN:HB3  | 9        | 0.22          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD11 | 14       | 0.22          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD12 | 14       | 0.22          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD13 | 14       | 0.22          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD21 | 14       | 0.22          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD22 | 14       | 0.22          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD23 | 14       | 0.22          |
| (1,814) | 1:A:21:GLU:HA   | 1:A:84:VAL:HG11 | 13       | 0.22          |
| (1,814) | 1:A:21:GLU:HA   | 1:A:84:VAL:HG12 | 13       | 0.22          |
| (1,814) | 1:A:21:GLU:HA   | 1:A:84:VAL:HG13 | 13       | 0.22          |
| (1,814) | 1:A:21:GLU:HA   | 1:A:84:VAL:HG21 | 13       | 0.22          |
| (1,814) | 1:A:21:GLU:HA   | 1:A:84:VAL:HG22 | 13       | 0.22          |
| (1,814) | 1:A:21:GLU:HA   | 1:A:84:VAL:HG23 | 13       | 0.22          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 4        | 0.22          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 4        | 0.22          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 4        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 4        | 0.22          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 5        | 0.22          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 5        | 0.22          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 5        | 0.22          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 5        | 0.22          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG11 | 2        | 0.22          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG12 | 2        | 0.22          |
| (1,734) | 1:A:47:PHE:HB3  | 1:A:87:VAL:HG13 | 2        | 0.22          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD11 | 10       | 0.22          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD12 | 10       | 0.22          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD13 | 10       | 0.22          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 11       | 0.22          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 2        | 0.22          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 2        | 0.22          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 2        | 0.22          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 3        | 0.22          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 3        | 0.22          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 3        | 0.22          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 8        | 0.22          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 8        | 0.22          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 8        | 0.22          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 11       | 0.22          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 18       | 0.22          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 6        | 0.22          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 16       | 0.22          |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB   | 6        | 0.22          |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB   | 15       | 0.22          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 14       | 0.22          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 14       | 0.22          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 14       | 0.22          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 14       | 0.22          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 14       | 0.22          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 14       | 0.22          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD1  | 6        | 0.22          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD2  | 6        | 0.22          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD1  | 8        | 0.22          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD2  | 8        | 0.22          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD1  | 16       | 0.22          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD2  | 16       | 0.22          |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 17       | 0.22          |
| (1,163) | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE1  | 4        | 0.22          |
| (1,163) | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE2  | 4        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 14       | 0.22          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 14       | 0.22          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 15       | 0.22          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 15       | 0.22          |
| (1,131) | 1:A:55:TYR:HD1  | 1:A:83:LEU:HG   | 14       | 0.22          |
| (1,131) | 1:A:55:TYR:HD2  | 1:A:83:LEU:HG   | 14       | 0.22          |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 6        | 0.22          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 10       | 0.21          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 10       | 0.21          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 10       | 0.21          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 10       | 0.21          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 10       | 0.21          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 10       | 0.21          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 13       | 0.21          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 13       | 0.21          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 13       | 0.21          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 13       | 0.21          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 13       | 0.21          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 13       | 0.21          |
| (1,903) | 1:A:53:LEU:HD11 | 1:A:87:VAL:HG11 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD11 | 1:A:87:VAL:HG12 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD11 | 1:A:87:VAL:HG13 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD12 | 1:A:87:VAL:HG11 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD12 | 1:A:87:VAL:HG12 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD12 | 1:A:87:VAL:HG13 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD13 | 1:A:87:VAL:HG11 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD13 | 1:A:87:VAL:HG12 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD13 | 1:A:87:VAL:HG13 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD21 | 1:A:87:VAL:HG11 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD21 | 1:A:87:VAL:HG12 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD21 | 1:A:87:VAL:HG13 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD22 | 1:A:87:VAL:HG11 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD22 | 1:A:87:VAL:HG12 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD22 | 1:A:87:VAL:HG13 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD23 | 1:A:87:VAL:HG11 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD23 | 1:A:87:VAL:HG12 | 17       | 0.21          |
| (1,903) | 1:A:53:LEU:HD23 | 1:A:87:VAL:HG13 | 17       | 0.21          |
| (1,888) | 1:A:52:GLY:HA3  | 1:A:88:ASN:HB2  | 1        | 0.21          |
| (1,888) | 1:A:52:GLY:HA3  | 1:A:88:ASN:HB3  | 1        | 0.21          |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA   | 15       | 0.21          |
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 15       | 0.21          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 10       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 10       | 0.21          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 10       | 0.21          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 10       | 0.21          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 14       | 0.21          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 14       | 0.21          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 14       | 0.21          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 14       | 0.21          |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB1  | 14       | 0.21          |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB2  | 14       | 0.21          |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB3  | 14       | 0.21          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 13       | 0.21          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 13       | 0.21          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 13       | 0.21          |
| (1,699) | 1:A:30:ILE:HG12 | 1:A:46:GLN:HG2  | 5        | 0.21          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 9        | 0.21          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB1  | 12       | 0.21          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB2  | 12       | 0.21          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB3  | 12       | 0.21          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 1        | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 1        | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 1        | 0.21          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 7        | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 7        | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 7        | 0.21          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 9        | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 9        | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 9        | 0.21          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 14       | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 14       | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 14       | 0.21          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 15       | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 15       | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 15       | 0.21          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 16       | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 16       | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 16       | 0.21          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 17       | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 17       | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 17       | 0.21          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 19       | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 19       | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 19       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 20       | 0.21          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 20       | 0.21          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 20       | 0.21          |
| (1,625) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HA   | 16       | 0.21          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 1        | 0.21          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 6        | 0.21          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 7        | 0.21          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 1        | 0.21          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 14       | 0.21          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 5        | 0.21          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 7        | 0.21          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 17       | 0.21          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 20       | 0.21          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB1  | 6        | 0.21          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB2  | 6        | 0.21          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB3  | 6        | 0.21          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 19       | 0.21          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 19       | 0.21          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 19       | 0.21          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 19       | 0.21          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 19       | 0.21          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 19       | 0.21          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 14       | 0.21          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 14       | 0.21          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 14       | 0.21          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 5        | 0.21          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 5        | 0.21          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 15       | 0.2           |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 15       | 0.2           |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 15       | 0.2           |
| (1,902) | 1:A:53:LEU:HD11 | 1:A:87:VAL:HA   | 17       | 0.2           |
| (1,902) | 1:A:53:LEU:HD12 | 1:A:87:VAL:HA   | 17       | 0.2           |
| (1,902) | 1:A:53:LEU:HD13 | 1:A:87:VAL:HA   | 17       | 0.2           |
| (1,902) | 1:A:53:LEU:HD21 | 1:A:87:VAL:HA   | 17       | 0.2           |
| (1,902) | 1:A:53:LEU:HD22 | 1:A:87:VAL:HA   | 17       | 0.2           |
| (1,902) | 1:A:53:LEU:HD23 | 1:A:87:VAL:HA   | 17       | 0.2           |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD11 | 6        | 0.2           |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD12 | 6        | 0.2           |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD13 | 6        | 0.2           |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD21 | 6        | 0.2           |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD22 | 6        | 0.2           |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD23 | 6        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,840) | 1:A:33:GLU:HB2  | 1:A:39:LEU:H    | 1        | 0.2           |
| (1,840) | 1:A:33:GLU:HB3  | 1:A:39:LEU:H    | 1        | 0.2           |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA   | 7        | 0.2           |
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 7        | 0.2           |
| (1,805) | 1:A:18:ARG:HB2  | 1:A:80:TRP:HB3  | 8        | 0.2           |
| (1,805) | 1:A:18:ARG:HB3  | 1:A:80:TRP:HB3  | 8        | 0.2           |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB1  | 12       | 0.2           |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB2  | 12       | 0.2           |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB3  | 12       | 0.2           |
| (1,749) | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 8        | 0.2           |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 19       | 0.2           |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 19       | 0.2           |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 19       | 0.2           |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 19       | 0.2           |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 19       | 0.2           |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 19       | 0.2           |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 19       | 0.2           |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 19       | 0.2           |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 19       | 0.2           |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 12       | 0.2           |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 12       | 0.2           |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 12       | 0.2           |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 6        | 0.2           |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 6        | 0.2           |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 12       | 0.2           |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 12       | 0.2           |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 12       | 0.2           |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 5        | 0.2           |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 9        | 0.2           |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 3        | 0.2           |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 5        | 0.2           |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 7        | 0.2           |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 11       | 0.2           |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 12       | 0.2           |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 15       | 0.2           |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 18       | 0.2           |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 19       | 0.2           |
| (1,496) | 1:A:32:SER:HB3  | 1:A:80:TRP:HD1  | 11       | 0.2           |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB   | 18       | 0.2           |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 6        | 0.2           |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 6        | 0.2           |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 6        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 6        | 0.2           |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 6        | 0.2           |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 6        | 0.2           |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 7        | 0.2           |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 7        | 0.2           |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 11       | 0.19          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 11       | 0.19          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 11       | 0.19          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 11       | 0.19          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 11       | 0.19          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 11       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD11 | 15       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD12 | 15       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD13 | 15       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD21 | 15       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD22 | 15       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD23 | 15       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD11 | 18       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD12 | 18       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD13 | 18       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD21 | 18       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD22 | 18       | 0.19          |
| (1,886) | 1:A:52:GLY:HA3  | 1:A:53:LEU:HD23 | 18       | 0.19          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 15       | 0.19          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 15       | 0.19          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 15       | 0.19          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 15       | 0.19          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 3        | 0.19          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 3        | 0.19          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 3        | 0.19          |
| (1,688) | 1:A:40:LEU:HB2  | 1:A:43:VAL:HG21 | 19       | 0.19          |
| (1,688) | 1:A:40:LEU:HB2  | 1:A:43:VAL:HG22 | 19       | 0.19          |
| (1,688) | 1:A:40:LEU:HB2  | 1:A:43:VAL:HG23 | 19       | 0.19          |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2  | 8        | 0.19          |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2  | 17       | 0.19          |
| (1,613) | 1:A:23:GLU:HA   | 1:A:84:VAL:HB   | 2        | 0.19          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 2        | 0.19          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 4        | 0.19          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 9        | 0.19          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 10       | 0.19          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 13       | 0.19          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3  | 17       | 0.19          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,487) | 1:A:84:VAL:H    | 1:A:84:VAL:HB  | 13       | 0.19          |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB  | 7        | 0.19          |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1 | 10       | 0.19          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1 | 4        | 0.19          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2 | 4        | 0.19          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1 | 20       | 0.19          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2 | 20       | 0.19          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1 | 6        | 0.18          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2 | 6        | 0.18          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3 | 6        | 0.18          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1 | 7        | 0.18          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2 | 7        | 0.18          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3 | 7        | 0.18          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1 | 9        | 0.18          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2 | 9        | 0.18          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3 | 9        | 0.18          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3 | 1        | 0.18          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3 | 7        | 0.18          |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2 | 16       | 0.18          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA  | 2        | 0.18          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA  | 20       | 0.18          |
| (1,642) | 1:A:78:ALA:HB1  | 1:A:79:GLY:HA3 | 6        | 0.18          |
| (1,642) | 1:A:78:ALA:HB2  | 1:A:79:GLY:HA3 | 6        | 0.18          |
| (1,642) | 1:A:78:ALA:HB3  | 1:A:79:GLY:HA3 | 6        | 0.18          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA  | 5        | 0.18          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA  | 5        | 0.18          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA  | 5        | 0.18          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA  | 11       | 0.18          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA  | 11       | 0.18          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA  | 11       | 0.18          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA  | 18       | 0.18          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA  | 18       | 0.18          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA  | 18       | 0.18          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3 | 15       | 0.18          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3 | 16       | 0.18          |
| (1,568) | 1:A:78:ALA:H    | 1:A:79:GLY:HA3 | 20       | 0.18          |
| (1,556) | 1:A:40:LEU:HB3  | 1:A:41:SER:HA  | 18       | 0.18          |
| (1,496) | 1:A:32:SER:HB3  | 1:A:80:TRP:HD1 | 1        | 0.18          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB  | 15       | 0.18          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB  | 19       | 0.18          |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB  | 3        | 0.18          |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB  | 3        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,273)  | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 17       | 0.18          |
| (1,273)  | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 17       | 0.18          |
| (1,273)  | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 17       | 0.18          |
| (1,273)  | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 17       | 0.18          |
| (1,273)  | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 17       | 0.18          |
| (1,273)  | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 17       | 0.18          |
| (1,219)  | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 1        | 0.18          |
| (1,219)  | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 1        | 0.18          |
| (1,219)  | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 1        | 0.18          |
| (1,190)  | 1:A:89:TYR:HA   | 1:A:89:TYR:HD1  | 13       | 0.18          |
| (1,190)  | 1:A:89:TYR:HA   | 1:A:89:TYR:HD2  | 13       | 0.18          |
| (1,186)  | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 3        | 0.18          |
| (1,186)  | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 20       | 0.18          |
| (1,163)  | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE1  | 3        | 0.18          |
| (1,163)  | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE2  | 3        | 0.18          |
| (1,163)  | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE1  | 19       | 0.18          |
| (1,163)  | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE2  | 19       | 0.18          |
| (1,163)  | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE1  | 20       | 0.18          |
| (1,163)  | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE2  | 20       | 0.18          |
| (1,156)  | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 1        | 0.18          |
| (1,156)  | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 1        | 0.18          |
| (1,135)  | 1:A:53:LEU:HG   | 1:A:85:TYR:HE1  | 15       | 0.18          |
| (1,135)  | 1:A:53:LEU:HG   | 1:A:85:TYR:HE2  | 15       | 0.18          |
| (1,135)  | 1:A:53:LEU:HG   | 1:A:85:TYR:HE1  | 18       | 0.18          |
| (1,135)  | 1:A:53:LEU:HG   | 1:A:85:TYR:HE2  | 18       | 0.18          |
| (1,104)  | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 2        | 0.18          |
| (1,104)  | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 5        | 0.18          |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD11 | 18       | 0.18          |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD12 | 18       | 0.18          |
| (1,1000) | 1:A:70:GLU:HB2  | 1:A:72:ILE:HD13 | 18       | 0.18          |
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD11 | 18       | 0.18          |
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD12 | 18       | 0.18          |
| (1,1000) | 1:A:70:GLU:HB3  | 1:A:72:ILE:HD13 | 18       | 0.18          |
| (1,990)  | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 1        | 0.17          |
| (1,990)  | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 1        | 0.17          |
| (1,990)  | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 1        | 0.17          |
| (1,990)  | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 1        | 0.17          |
| (1,990)  | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 1        | 0.17          |
| (1,990)  | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 1        | 0.17          |
| (1,990)  | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 20       | 0.17          |
| (1,990)  | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 20       | 0.17          |
| (1,990)  | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 20       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 20       | 0.17          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 20       | 0.17          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 20       | 0.17          |
| (1,938) | 1:A:57:ASN:HD21 | 1:A:60:SER:H    | 5        | 0.17          |
| (1,938) | 1:A:57:ASN:HD22 | 1:A:60:SER:H    | 5        | 0.17          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 14       | 0.17          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 14       | 0.17          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 14       | 0.17          |
| (1,840) | 1:A:33:GLU:HB2  | 1:A:39:LEU:H    | 19       | 0.17          |
| (1,840) | 1:A:33:GLU:HB3  | 1:A:39:LEU:H    | 19       | 0.17          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 19       | 0.17          |
| (1,795) | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 19       | 0.17          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 19       | 0.17          |
| (1,795) | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 19       | 0.17          |
| (1,790) | 1:A:15:GLU:HB2  | 1:A:36:GLY:HA3  | 1        | 0.17          |
| (1,790) | 1:A:15:GLU:HB3  | 1:A:36:GLY:HA3  | 1        | 0.17          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 6        | 0.17          |
| (1,637) | 1:A:30:ILE:HD11 | 1:A:43:VAL:HA   | 4        | 0.17          |
| (1,637) | 1:A:30:ILE:HD12 | 1:A:43:VAL:HA   | 4        | 0.17          |
| (1,637) | 1:A:30:ILE:HD13 | 1:A:43:VAL:HA   | 4        | 0.17          |
| (1,625) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HA   | 19       | 0.17          |
| (1,519) | 1:A:53:LEU:HA   | 1:A:87:VAL:HG11 | 2        | 0.17          |
| (1,519) | 1:A:53:LEU:HA   | 1:A:87:VAL:HG12 | 2        | 0.17          |
| (1,519) | 1:A:53:LEU:HA   | 1:A:87:VAL:HG13 | 2        | 0.17          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 11       | 0.17          |
| (1,354) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HB2  | 2        | 0.17          |
| (1,354) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HB3  | 2        | 0.17          |
| (1,354) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB2  | 2        | 0.17          |
| (1,354) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB3  | 2        | 0.17          |
| (1,354) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB2  | 2        | 0.17          |
| (1,354) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB3  | 2        | 0.17          |
| (1,354) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HB2  | 11       | 0.17          |
| (1,354) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HB3  | 11       | 0.17          |
| (1,354) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB2  | 11       | 0.17          |
| (1,354) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB3  | 11       | 0.17          |
| (1,354) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB2  | 11       | 0.17          |
| (1,354) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB3  | 11       | 0.17          |
| (1,350) | 1:A:17:ILE:HD11 | 1:A:30:ILE:HB   | 10       | 0.17          |
| (1,350) | 1:A:17:ILE:HD12 | 1:A:30:ILE:HB   | 10       | 0.17          |
| (1,350) | 1:A:17:ILE:HD13 | 1:A:30:ILE:HB   | 10       | 0.17          |
| (1,318) | 1:A:21:GLU:HA   | 1:A:87:VAL:HG11 | 13       | 0.17          |
| (1,318) | 1:A:21:GLU:HA   | 1:A:87:VAL:HG12 | 13       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,318) | 1:A:21:GLU:HA   | 1:A:87:VAL:HG13 | 13       | 0.17          |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB   | 14       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 8        | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 8        | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 8        | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 13       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 13       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 13       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 15       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 15       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 15       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 18       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 18       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 18       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 20       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 20       | 0.17          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 20       | 0.17          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 8        | 0.17          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 8        | 0.17          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 8        | 0.17          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 8        | 0.17          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 8        | 0.17          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 8        | 0.17          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD1  | 3        | 0.17          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD2  | 3        | 0.17          |
| (1,135) | 1:A:53:LEU:HG   | 1:A:85:TYR:HE1  | 14       | 0.17          |
| (1,135) | 1:A:53:LEU:HG   | 1:A:85:TYR:HE2  | 14       | 0.17          |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 9        | 0.17          |
| (1,967) | 1:A:66:VAL:HG11 | 1:A:85:TYR:HA   | 11       | 0.16          |
| (1,967) | 1:A:66:VAL:HG12 | 1:A:85:TYR:HA   | 11       | 0.16          |
| (1,967) | 1:A:66:VAL:HG13 | 1:A:85:TYR:HA   | 11       | 0.16          |
| (1,967) | 1:A:66:VAL:HG21 | 1:A:85:TYR:HA   | 11       | 0.16          |
| (1,967) | 1:A:66:VAL:HG22 | 1:A:85:TYR:HA   | 11       | 0.16          |
| (1,967) | 1:A:66:VAL:HG23 | 1:A:85:TYR:HA   | 11       | 0.16          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 8        | 0.16          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB2  | 8        | 0.16          |
| (1,92)  | 1:A:44:THR:H    | 1:A:50:ALA:HB3  | 8        | 0.16          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG11 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG12 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG13 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG21 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG22 | 9        | 0.16          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,919) | 1:A:55:TYR:HD1 | 1:A:66:VAL:HG23 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG11 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG12 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG13 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG21 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG22 | 9        | 0.16          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG23 | 9        | 0.16          |
| (1,795) | 1:A:16:TYR:HE1 | 1:A:82:ASN:HD21 | 13       | 0.16          |
| (1,795) | 1:A:16:TYR:HE1 | 1:A:82:ASN:HD22 | 13       | 0.16          |
| (1,795) | 1:A:16:TYR:HE2 | 1:A:82:ASN:HD21 | 13       | 0.16          |
| (1,795) | 1:A:16:TYR:HE2 | 1:A:82:ASN:HD22 | 13       | 0.16          |
| (1,668) | 1:A:75:ALA:HB1 | 1:A:76:PRO:HD3  | 19       | 0.16          |
| (1,668) | 1:A:75:ALA:HB2 | 1:A:76:PRO:HD3  | 19       | 0.16          |
| (1,668) | 1:A:75:ALA:HB3 | 1:A:76:PRO:HD3  | 19       | 0.16          |
| (1,645) | 1:A:32:SER:HB3 | 1:A:38:VAL:HA   | 17       | 0.16          |
| (1,627) | 1:A:21:GLU:HG3 | 1:A:87:VAL:HA   | 8        | 0.16          |
| (1,589) | 1:A:70:GLU:H   | 1:A:71:GLY:HA3  | 16       | 0.16          |
| (1,577) | 1:A:55:TYR:HE1 | 1:A:76:PRO:HA   | 16       | 0.16          |
| (1,577) | 1:A:55:TYR:HE2 | 1:A:76:PRO:HA   | 16       | 0.16          |
| (1,576) | 1:A:56:ARG:HA  | 1:A:56:ARG:HE   | 11       | 0.16          |
| (1,563) | 1:A:36:GLY:HA3 | 1:A:80:TRP:HE1  | 14       | 0.16          |
| (1,486) | 1:A:83:LEU:HG  | 1:A:84:VAL:H    | 3        | 0.16          |
| (1,486) | 1:A:83:LEU:HG  | 1:A:84:VAL:H    | 9        | 0.16          |
| (1,405) | 1:A:55:TYR:H   | 1:A:86:VAL:HB   | 3        | 0.16          |
| (1,391) | 1:A:33:GLU:H   | 1:A:38:VAL:HG11 | 8        | 0.16          |
| (1,391) | 1:A:33:GLU:H   | 1:A:38:VAL:HG12 | 8        | 0.16          |
| (1,391) | 1:A:33:GLU:H   | 1:A:38:VAL:HG13 | 8        | 0.16          |
| (1,354) | 1:A:75:ALA:HB1 | 1:A:76:PRO:HB2  | 4        | 0.16          |
| (1,354) | 1:A:75:ALA:HB1 | 1:A:76:PRO:HB3  | 4        | 0.16          |
| (1,354) | 1:A:75:ALA:HB2 | 1:A:76:PRO:HB2  | 4        | 0.16          |
| (1,354) | 1:A:75:ALA:HB2 | 1:A:76:PRO:HB3  | 4        | 0.16          |
| (1,354) | 1:A:75:ALA:HB3 | 1:A:76:PRO:HB2  | 4        | 0.16          |
| (1,354) | 1:A:75:ALA:HB3 | 1:A:76:PRO:HB3  | 4        | 0.16          |
| (1,354) | 1:A:75:ALA:HB1 | 1:A:76:PRO:HB2  | 12       | 0.16          |
| (1,354) | 1:A:75:ALA:HB1 | 1:A:76:PRO:HB3  | 12       | 0.16          |
| (1,354) | 1:A:75:ALA:HB2 | 1:A:76:PRO:HB2  | 12       | 0.16          |
| (1,354) | 1:A:75:ALA:HB2 | 1:A:76:PRO:HB3  | 12       | 0.16          |
| (1,354) | 1:A:75:ALA:HB3 | 1:A:76:PRO:HB2  | 12       | 0.16          |
| (1,354) | 1:A:75:ALA:HB3 | 1:A:76:PRO:HB3  | 12       | 0.16          |
| (1,354) | 1:A:75:ALA:HB1 | 1:A:76:PRO:HB2  | 13       | 0.16          |
| (1,354) | 1:A:75:ALA:HB1 | 1:A:76:PRO:HB3  | 13       | 0.16          |
| (1,354) | 1:A:75:ALA:HB2 | 1:A:76:PRO:HB2  | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,354)  | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB3  | 13       | 0.16          |
| (1,354)  | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB2  | 13       | 0.16          |
| (1,354)  | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB3  | 13       | 0.16          |
| (1,323)  | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 11       | 0.16          |
| (1,323)  | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 11       | 0.16          |
| (1,323)  | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 11       | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 6        | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 6        | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 6        | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 12       | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 12       | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 12       | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 19       | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 19       | 0.16          |
| (1,306)  | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 19       | 0.16          |
| (1,303)  | 1:A:28:ILE:HG21 | 1:A:46:GLN:HG3  | 7        | 0.16          |
| (1,303)  | 1:A:28:ILE:HG22 | 1:A:46:GLN:HG3  | 7        | 0.16          |
| (1,303)  | 1:A:28:ILE:HG23 | 1:A:46:GLN:HG3  | 7        | 0.16          |
| (1,273)  | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 8        | 0.16          |
| (1,273)  | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 8        | 0.16          |
| (1,273)  | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 8        | 0.16          |
| (1,273)  | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 8        | 0.16          |
| (1,273)  | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 8        | 0.16          |
| (1,273)  | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 8        | 0.16          |
| (1,273)  | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 16       | 0.16          |
| (1,273)  | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 16       | 0.16          |
| (1,273)  | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 16       | 0.16          |
| (1,273)  | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 16       | 0.16          |
| (1,273)  | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 16       | 0.16          |
| (1,273)  | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 16       | 0.16          |
| (1,171)  | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 11       | 0.16          |
| (1,171)  | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 11       | 0.16          |
| (1,154)  | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 10       | 0.16          |
| (1,154)  | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 10       | 0.16          |
| (1,135)  | 1:A:53:LEU:HG   | 1:A:85:TYR:HE1  | 6        | 0.16          |
| (1,135)  | 1:A:53:LEU:HG   | 1:A:85:TYR:HE2  | 6        | 0.16          |
| (1,104)  | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 11       | 0.16          |
| (1,1019) | 1:A:87:VAL:HA   | 1:A:88:ASN:HB2  | 2        | 0.16          |
| (1,1019) | 1:A:87:VAL:HA   | 1:A:88:ASN:HB3  | 2        | 0.16          |
| (1,938)  | 1:A:57:ASN:HD21 | 1:A:60:SER:H    | 16       | 0.15          |
| (1,938)  | 1:A:57:ASN:HD22 | 1:A:60:SER:H    | 16       | 0.15          |
| (1,92)   | 1:A:44:THR:H    | 1:A:50:ALA:HB1  | 16       | 0.15          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,92)  | 1:A:44:THR:H   | 1:A:50:ALA:HB2  | 16       | 0.15          |
| (1,92)  | 1:A:44:THR:H   | 1:A:50:ALA:HB3  | 16       | 0.15          |
| (1,919) | 1:A:55:TYR:HD1 | 1:A:66:VAL:HG11 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD1 | 1:A:66:VAL:HG12 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD1 | 1:A:66:VAL:HG13 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD1 | 1:A:66:VAL:HG21 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD1 | 1:A:66:VAL:HG22 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD1 | 1:A:66:VAL:HG23 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG11 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG12 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG13 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG21 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG22 | 2        | 0.15          |
| (1,919) | 1:A:55:TYR:HD2 | 1:A:66:VAL:HG23 | 2        | 0.15          |
| (1,885) | 1:A:52:GLY:H   | 1:A:88:ASN:HB2  | 9        | 0.15          |
| (1,885) | 1:A:52:GLY:H   | 1:A:88:ASN:HB3  | 9        | 0.15          |
| (1,750) | 1:A:30:ILE:HB  | 1:A:45:ALA:HB1  | 15       | 0.15          |
| (1,750) | 1:A:30:ILE:HB  | 1:A:45:ALA:HB2  | 15       | 0.15          |
| (1,750) | 1:A:30:ILE:HB  | 1:A:45:ALA:HB3  | 15       | 0.15          |
| (1,688) | 1:A:40:LEU:HB2 | 1:A:43:VAL:HG21 | 2        | 0.15          |
| (1,688) | 1:A:40:LEU:HB2 | 1:A:43:VAL:HG22 | 2        | 0.15          |
| (1,688) | 1:A:40:LEU:HB2 | 1:A:43:VAL:HG23 | 2        | 0.15          |
| (1,670) | 1:A:40:LEU:HB2 | 1:A:43:VAL:HB   | 19       | 0.15          |
| (1,668) | 1:A:75:ALA:HB1 | 1:A:76:PRO:HD3  | 5        | 0.15          |
| (1,668) | 1:A:75:ALA:HB2 | 1:A:76:PRO:HD3  | 5        | 0.15          |
| (1,668) | 1:A:75:ALA:HB3 | 1:A:76:PRO:HD3  | 5        | 0.15          |
| (1,642) | 1:A:78:ALA:HB1 | 1:A:79:GLY:HA3  | 1        | 0.15          |
| (1,642) | 1:A:78:ALA:HB2 | 1:A:79:GLY:HA3  | 1        | 0.15          |
| (1,642) | 1:A:78:ALA:HB3 | 1:A:79:GLY:HA3  | 1        | 0.15          |
| (1,589) | 1:A:70:GLU:H   | 1:A:71:GLY:HA3  | 3        | 0.15          |
| (1,589) | 1:A:70:GLU:H   | 1:A:71:GLY:HA3  | 5        | 0.15          |
| (1,589) | 1:A:70:GLU:H   | 1:A:71:GLY:HA3  | 9        | 0.15          |
| (1,589) | 1:A:70:GLU:H   | 1:A:71:GLY:HA3  | 11       | 0.15          |
| (1,589) | 1:A:70:GLU:H   | 1:A:71:GLY:HA3  | 19       | 0.15          |
| (1,569) | 1:A:52:GLY:HA3 | 1:A:88:ASN:H    | 7        | 0.15          |
| (1,556) | 1:A:40:LEU:HB3 | 1:A:41:SER:HA   | 6        | 0.15          |
| (1,556) | 1:A:40:LEU:HB3 | 1:A:41:SER:HA   | 15       | 0.15          |
| (1,486) | 1:A:83:LEU:HG  | 1:A:84:VAL:H    | 2        | 0.15          |
| (1,486) | 1:A:83:LEU:HG  | 1:A:84:VAL:H    | 11       | 0.15          |
| (1,486) | 1:A:83:LEU:HG  | 1:A:84:VAL:H    | 15       | 0.15          |
| (1,405) | 1:A:55:TYR:H   | 1:A:86:VAL:HB   | 12       | 0.15          |
| (1,405) | 1:A:55:TYR:H   | 1:A:86:VAL:HB   | 17       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,354) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HB2  | 20       | 0.15          |
| (1,354) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HB3  | 20       | 0.15          |
| (1,354) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB2  | 20       | 0.15          |
| (1,354) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HB3  | 20       | 0.15          |
| (1,354) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB2  | 20       | 0.15          |
| (1,354) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HB3  | 20       | 0.15          |
| (1,346) | 1:A:55:TYR:HD1  | 1:A:56:ARG:HA   | 17       | 0.15          |
| (1,346) | 1:A:55:TYR:HD2  | 1:A:56:ARG:HA   | 17       | 0.15          |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB   | 16       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 5        | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 5        | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 5        | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 7        | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 7        | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 7        | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 11       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 11       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 11       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 14       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 14       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 14       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG11 | 16       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG12 | 16       | 0.15          |
| (1,306) | 1:A:47:PHE:HB2  | 1:A:87:VAL:HG13 | 16       | 0.15          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 1        | 0.15          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 1        | 0.15          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 1        | 0.15          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 1        | 0.15          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 1        | 0.15          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 1        | 0.15          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 11       | 0.15          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 11       | 0.15          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 11       | 0.15          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 11       | 0.15          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 11       | 0.15          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 11       | 0.15          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 12       | 0.15          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 12       | 0.15          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 12       | 0.15          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 12       | 0.15          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 12       | 0.15          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 12       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,269) | 1:A:19:VAL:HA   | 1:A:28:ILE:HG21 | 10       | 0.15          |
| (1,269) | 1:A:19:VAL:HA   | 1:A:28:ILE:HG22 | 10       | 0.15          |
| (1,269) | 1:A:19:VAL:HA   | 1:A:28:ILE:HG23 | 10       | 0.15          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 11       | 0.15          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 11       | 0.15          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 11       | 0.15          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 10       | 0.15          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 10       | 0.15          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE1  | 14       | 0.15          |
| (1,171) | 1:A:46:GLN:HG2  | 1:A:47:PHE:HE2  | 14       | 0.15          |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 3        | 0.15          |
| (1,104) | 1:A:39:LEU:H    | 1:A:72:ILE:HA   | 7        | 0.15          |
| (1,967) | 1:A:66:VAL:HG11 | 1:A:85:TYR:HA   | 2        | 0.14          |
| (1,967) | 1:A:66:VAL:HG12 | 1:A:85:TYR:HA   | 2        | 0.14          |
| (1,967) | 1:A:66:VAL:HG13 | 1:A:85:TYR:HA   | 2        | 0.14          |
| (1,967) | 1:A:66:VAL:HG21 | 1:A:85:TYR:HA   | 2        | 0.14          |
| (1,967) | 1:A:66:VAL:HG22 | 1:A:85:TYR:HA   | 2        | 0.14          |
| (1,967) | 1:A:66:VAL:HG23 | 1:A:85:TYR:HA   | 2        | 0.14          |
| (1,967) | 1:A:66:VAL:HG11 | 1:A:85:TYR:HA   | 9        | 0.14          |
| (1,967) | 1:A:66:VAL:HG12 | 1:A:85:TYR:HA   | 9        | 0.14          |
| (1,967) | 1:A:66:VAL:HG13 | 1:A:85:TYR:HA   | 9        | 0.14          |
| (1,967) | 1:A:66:VAL:HG21 | 1:A:85:TYR:HA   | 9        | 0.14          |
| (1,967) | 1:A:66:VAL:HG22 | 1:A:85:TYR:HA   | 9        | 0.14          |
| (1,967) | 1:A:66:VAL:HG23 | 1:A:85:TYR:HA   | 9        | 0.14          |
| (1,912) | 1:A:54:ARG:HD2  | 1:A:65:GLY:HA2  | 18       | 0.14          |
| (1,912) | 1:A:54:ARG:HD2  | 1:A:65:GLY:HA3  | 18       | 0.14          |
| (1,912) | 1:A:54:ARG:HD3  | 1:A:65:GLY:HA2  | 18       | 0.14          |
| (1,912) | 1:A:54:ARG:HD3  | 1:A:65:GLY:HA3  | 18       | 0.14          |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 3        | 0.14          |
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 3        | 0.14          |
| (1,839) | 1:A:33:GLU:HB2  | 1:A:38:VAL:HA   | 5        | 0.14          |
| (1,839) | 1:A:33:GLU:HB3  | 1:A:38:VAL:HA   | 5        | 0.14          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG11 | 9        | 0.14          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG12 | 9        | 0.14          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG13 | 9        | 0.14          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG21 | 9        | 0.14          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG22 | 9        | 0.14          |
| (1,815) | 1:A:21:GLU:HG2  | 1:A:84:VAL:HG23 | 9        | 0.14          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 16       | 0.14          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 16       | 0.14          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 16       | 0.14          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 16       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 16       | 0.14          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 16       | 0.14          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 16       | 0.14          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 16       | 0.14          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 16       | 0.14          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD11 | 11       | 0.14          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD12 | 11       | 0.14          |
| (1,721) | 1:A:71:GLY:HA3  | 1:A:72:ILE:HD13 | 11       | 0.14          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 2        | 0.14          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 2        | 0.14          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 2        | 0.14          |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 16       | 0.14          |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 16       | 0.14          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 11       | 0.14          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 14       | 0.14          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 18       | 0.14          |
| (1,668) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HD3  | 11       | 0.14          |
| (1,668) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HD3  | 11       | 0.14          |
| (1,668) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HD3  | 11       | 0.14          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 19       | 0.14          |
| (1,643) | 1:A:17:ILE:HG21 | 1:A:32:SER:HB3  | 4        | 0.14          |
| (1,643) | 1:A:17:ILE:HG22 | 1:A:32:SER:HB3  | 4        | 0.14          |
| (1,643) | 1:A:17:ILE:HG23 | 1:A:32:SER:HB3  | 4        | 0.14          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB1  | 15       | 0.14          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB2  | 15       | 0.14          |
| (1,641) | 1:A:43:VAL:HA   | 1:A:45:ALA:HB3  | 15       | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 1        | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 2        | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 4        | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 6        | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 8        | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 10       | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 12       | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 13       | 0.14          |
| (1,589) | 1:A:70:GLU:H    | 1:A:71:GLY:HA3  | 14       | 0.14          |
| (1,569) | 1:A:52:GLY:HA3  | 1:A:88:ASN:H    | 20       | 0.14          |
| (1,563) | 1:A:36:GLY:HA3  | 1:A:80:TRP:HE1  | 15       | 0.14          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 16       | 0.14          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 19       | 0.14          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 20       | 0.14          |
| (1,425) | 1:A:41:SER:H    | 1:A:43:VAL:HB   | 4        | 0.14          |
| (1,323) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 2        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,323) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 2        | 0.14          |
| (1,323) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 2        | 0.14          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 9        | 0.14          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 9        | 0.14          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 9        | 0.14          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 9        | 0.14          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 9        | 0.14          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 9        | 0.14          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 5        | 0.14          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 5        | 0.14          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 5        | 0.14          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 5        | 0.14          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 5        | 0.14          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 5        | 0.14          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE1  | 7        | 0.14          |
| (1,273) | 1:A:43:VAL:HG11 | 1:A:47:PHE:HE2  | 7        | 0.14          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE1  | 7        | 0.14          |
| (1,273) | 1:A:43:VAL:HG12 | 1:A:47:PHE:HE2  | 7        | 0.14          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE1  | 7        | 0.14          |
| (1,273) | 1:A:43:VAL:HG13 | 1:A:47:PHE:HE2  | 7        | 0.14          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 16       | 0.14          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 16       | 0.14          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 18       | 0.14          |
| (1,156) | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 18       | 0.14          |
| (1,990) | 1:A:68:LEU:HD11 | 1:A:73:LEU:HG   | 7        | 0.13          |
| (1,990) | 1:A:68:LEU:HD12 | 1:A:73:LEU:HG   | 7        | 0.13          |
| (1,990) | 1:A:68:LEU:HD13 | 1:A:73:LEU:HG   | 7        | 0.13          |
| (1,990) | 1:A:68:LEU:HD21 | 1:A:73:LEU:HG   | 7        | 0.13          |
| (1,990) | 1:A:68:LEU:HD22 | 1:A:73:LEU:HG   | 7        | 0.13          |
| (1,990) | 1:A:68:LEU:HD23 | 1:A:73:LEU:HG   | 7        | 0.13          |
| (1,910) | 1:A:54:ARG:HG2  | 1:A:55:TYR:H    | 14       | 0.13          |
| (1,910) | 1:A:54:ARG:HG3  | 1:A:55:TYR:H    | 14       | 0.13          |
| (1,885) | 1:A:52:GLY:H    | 1:A:88:ASN:HB2  | 1        | 0.13          |
| (1,885) | 1:A:52:GLY:H    | 1:A:88:ASN:HB3  | 1        | 0.13          |
| (1,841) | 1:A:35:ASP:HB2  | 1:A:36:GLY:HA3  | 6        | 0.13          |
| (1,841) | 1:A:35:ASP:HB3  | 1:A:36:GLY:HA3  | 6        | 0.13          |
| (1,746) | 1:A:40:LEU:HA   | 1:A:71:GLY:HA3  | 4        | 0.13          |
| (1,746) | 1:A:40:LEU:HA   | 1:A:71:GLY:HA3  | 18       | 0.13          |
| (1,746) | 1:A:40:LEU:HA   | 1:A:71:GLY:HA3  | 20       | 0.13          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG21 | 13       | 0.13          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG22 | 13       | 0.13          |
| (1,733) | 1:A:86:VAL:HG11 | 1:A:87:VAL:HG23 | 13       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG21 | 13       | 0.13          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG22 | 13       | 0.13          |
| (1,733) | 1:A:86:VAL:HG12 | 1:A:87:VAL:HG23 | 13       | 0.13          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG21 | 13       | 0.13          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG22 | 13       | 0.13          |
| (1,733) | 1:A:86:VAL:HG13 | 1:A:87:VAL:HG23 | 13       | 0.13          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB1  | 4        | 0.13          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB2  | 4        | 0.13          |
| (1,710) | 1:A:43:VAL:HG11 | 1:A:50:ALA:HB3  | 4        | 0.13          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB1  | 4        | 0.13          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB2  | 4        | 0.13          |
| (1,710) | 1:A:43:VAL:HG12 | 1:A:50:ALA:HB3  | 4        | 0.13          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB1  | 4        | 0.13          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB2  | 4        | 0.13          |
| (1,710) | 1:A:43:VAL:HG13 | 1:A:50:ALA:HB3  | 4        | 0.13          |
| (1,700) | 1:A:55:TYR:HB3  | 1:A:83:LEU:HG   | 7        | 0.13          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 3        | 0.13          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 4        | 0.13          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 5        | 0.13          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 12       | 0.13          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 15       | 0.13          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 19       | 0.13          |
| (1,668) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HD3  | 2        | 0.13          |
| (1,668) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HD3  | 2        | 0.13          |
| (1,668) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HD3  | 2        | 0.13          |
| (1,645) | 1:A:32:SER:HB3  | 1:A:38:VAL:HA   | 5        | 0.13          |
| (1,643) | 1:A:17:ILE:HG21 | 1:A:32:SER:HB3  | 11       | 0.13          |
| (1,643) | 1:A:17:ILE:HG22 | 1:A:32:SER:HB3  | 11       | 0.13          |
| (1,643) | 1:A:17:ILE:HG23 | 1:A:32:SER:HB3  | 11       | 0.13          |
| (1,556) | 1:A:40:LEU:HB3  | 1:A:41:SER:HA   | 3        | 0.13          |
| (1,556) | 1:A:40:LEU:HB3  | 1:A:41:SER:HA   | 7        | 0.13          |
| (1,486) | 1:A:83:LEU:HG   | 1:A:84:VAL:H    | 12       | 0.13          |
| (1,455) | 1:A:55:TYR:HA   | 1:A:66:VAL:H    | 7        | 0.13          |
| (1,455) | 1:A:55:TYR:HA   | 1:A:66:VAL:H    | 17       | 0.13          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 20       | 0.13          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB1  | 3        | 0.13          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB2  | 3        | 0.13          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB3  | 3        | 0.13          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB1  | 9        | 0.13          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB2  | 9        | 0.13          |
| (1,353) | 1:A:17:ILE:HB   | 1:A:75:ALA:HB3  | 9        | 0.13          |
| (1,323) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 12       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,323) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 12       | 0.13          |
| (1,323) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 12       | 0.13          |
| (1,323) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 13       | 0.13          |
| (1,323) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 13       | 0.13          |
| (1,323) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 13       | 0.13          |
| (1,310) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HB   | 8        | 0.13          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB1  | 10       | 0.13          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB2  | 10       | 0.13          |
| (1,300) | 1:A:76:PRO:HB2  | 1:A:78:ALA:HB3  | 10       | 0.13          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB1  | 10       | 0.13          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB2  | 10       | 0.13          |
| (1,300) | 1:A:76:PRO:HB3  | 1:A:78:ALA:HB3  | 10       | 0.13          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 15       | 0.13          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 15       | 0.13          |
| (1,234) | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 15       | 0.13          |
| (1,219) | 1:A:17:ILE:HD11 | 1:A:32:SER:HB3  | 4        | 0.13          |
| (1,219) | 1:A:17:ILE:HD12 | 1:A:32:SER:HB3  | 4        | 0.13          |
| (1,219) | 1:A:17:ILE:HD13 | 1:A:32:SER:HB3  | 4        | 0.13          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD1  | 19       | 0.13          |
| (1,190) | 1:A:89:TYR:HA   | 1:A:89:TYR:HD2  | 19       | 0.13          |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 5        | 0.13          |
| (1,186) | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 15       | 0.13          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD1  | 6        | 0.13          |
| (1,154) | 1:A:21:GLU:HB3  | 1:A:47:PHE:HD2  | 6        | 0.13          |
| (1,129) | 1:A:28:ILE:HG21 | 1:A:46:GLN:H    | 10       | 0.13          |
| (1,129) | 1:A:28:ILE:HG22 | 1:A:46:GLN:H    | 10       | 0.13          |
| (1,129) | 1:A:28:ILE:HG23 | 1:A:46:GLN:H    | 10       | 0.13          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG11 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG12 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG13 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG21 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG22 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD1  | 1:A:66:VAL:HG23 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG11 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG12 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG13 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG21 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG22 | 3        | 0.12          |
| (1,919) | 1:A:55:TYR:HD2  | 1:A:66:VAL:HG23 | 3        | 0.12          |
| (1,864) | 1:A:39:LEU:HB2  | 1:A:72:ILE:HG13 | 5        | 0.12          |
| (1,864) | 1:A:39:LEU:HB3  | 1:A:72:ILE:HG13 | 5        | 0.12          |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB1  | 18       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB2  | 18       | 0.12          |
| (1,750) | 1:A:30:ILE:HB   | 1:A:45:ALA:HB3  | 18       | 0.12          |
| (1,749) | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 1        | 0.12          |
| (1,749) | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 5        | 0.12          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG11 | 4        | 0.12          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG12 | 4        | 0.12          |
| (1,715) | 1:A:54:ARG:HB2  | 1:A:86:VAL:HG13 | 4        | 0.12          |
| (1,704) | 1:A:67:ARG:HG2  | 1:A:74:HIS:HA   | 3        | 0.12          |
| (1,704) | 1:A:67:ARG:HG3  | 1:A:74:HIS:HA   | 3        | 0.12          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 2        | 0.12          |
| (1,675) | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 9        | 0.12          |
| (1,668) | 1:A:75:ALA:HB1  | 1:A:76:PRO:HD3  | 4        | 0.12          |
| (1,668) | 1:A:75:ALA:HB2  | 1:A:76:PRO:HD3  | 4        | 0.12          |
| (1,668) | 1:A:75:ALA:HB3  | 1:A:76:PRO:HD3  | 4        | 0.12          |
| (1,656) | 1:A:54:ARG:HB3  | 1:A:85:TYR:HB2  | 2        | 0.12          |
| (1,643) | 1:A:17:ILE:HG21 | 1:A:32:SER:HB3  | 1        | 0.12          |
| (1,643) | 1:A:17:ILE:HG22 | 1:A:32:SER:HB3  | 1        | 0.12          |
| (1,643) | 1:A:17:ILE:HG23 | 1:A:32:SER:HB3  | 1        | 0.12          |
| (1,643) | 1:A:17:ILE:HG21 | 1:A:32:SER:HB3  | 13       | 0.12          |
| (1,643) | 1:A:17:ILE:HG22 | 1:A:32:SER:HB3  | 13       | 0.12          |
| (1,643) | 1:A:17:ILE:HG23 | 1:A:32:SER:HB3  | 13       | 0.12          |
| (1,625) | 1:A:21:GLU:HG2  | 1:A:87:VAL:HA   | 1        | 0.12          |
| (1,569) | 1:A:52:GLY:HA3  | 1:A:88:ASN:H    | 2        | 0.12          |
| (1,569) | 1:A:52:GLY:HA3  | 1:A:88:ASN:H    | 15       | 0.12          |
| (1,556) | 1:A:40:LEU:HB3  | 1:A:41:SER:HA   | 16       | 0.12          |
| (1,492) | 1:A:50:ALA:HB1  | 1:A:52:GLY:H    | 11       | 0.12          |
| (1,492) | 1:A:50:ALA:HB2  | 1:A:52:GLY:H    | 11       | 0.12          |
| (1,492) | 1:A:50:ALA:HB3  | 1:A:52:GLY:H    | 11       | 0.12          |
| (1,42)  | 1:A:87:VAL:HG11 | 1:A:88:ASN:H    | 19       | 0.12          |
| (1,42)  | 1:A:87:VAL:HG12 | 1:A:88:ASN:H    | 19       | 0.12          |
| (1,42)  | 1:A:87:VAL:HG13 | 1:A:88:ASN:H    | 19       | 0.12          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 2        | 0.12          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 5        | 0.12          |
| (1,405) | 1:A:55:TYR:H    | 1:A:86:VAL:HB   | 8        | 0.12          |
| (1,335) | 1:A:54:ARG:HB3  | 1:A:86:VAL:HB   | 12       | 0.12          |
| (1,323) | 1:A:75:ALA:HB1  | 1:A:79:GLY:HA3  | 20       | 0.12          |
| (1,323) | 1:A:75:ALA:HB2  | 1:A:79:GLY:HA3  | 20       | 0.12          |
| (1,323) | 1:A:75:ALA:HB3  | 1:A:79:GLY:HA3  | 20       | 0.12          |
| (1,317) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HG11 | 4        | 0.12          |
| (1,317) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HG12 | 4        | 0.12          |
| (1,317) | 1:A:21:GLU:HG3  | 1:A:87:VAL:HG13 | 4        | 0.12          |
| (1,311) | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB   | 11       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,311)  | 1:A:40:LEU:HB3  | 1:A:43:VAL:HB   | 13       | 0.12          |
| (1,245)  | 1:A:43:VAL:HA   | 1:A:46:GLN:HB2  | 8        | 0.12          |
| (1,234)  | 1:A:44:THR:HA   | 1:A:50:ALA:HB1  | 6        | 0.12          |
| (1,234)  | 1:A:44:THR:HA   | 1:A:50:ALA:HB2  | 6        | 0.12          |
| (1,234)  | 1:A:44:THR:HA   | 1:A:50:ALA:HB3  | 6        | 0.12          |
| (1,190)  | 1:A:89:TYR:HA   | 1:A:89:TYR:HD1  | 1        | 0.12          |
| (1,190)  | 1:A:89:TYR:HA   | 1:A:89:TYR:HD2  | 1        | 0.12          |
| (1,186)  | 1:A:32:SER:HB2  | 1:A:80:TRP:HD1  | 6        | 0.12          |
| (1,163)  | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE1  | 18       | 0.12          |
| (1,163)  | 1:A:21:GLU:HB3  | 1:A:85:TYR:HE2  | 18       | 0.12          |
| (1,156)  | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE1  | 15       | 0.12          |
| (1,156)  | 1:A:46:GLN:HG3  | 1:A:47:PHE:HE2  | 15       | 0.12          |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG11 | 19       | 0.12          |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG12 | 19       | 0.12          |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG13 | 19       | 0.12          |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG21 | 19       | 0.12          |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG22 | 19       | 0.12          |
| (1,1011) | 1:A:83:LEU:HA   | 1:A:84:VAL:HG23 | 19       | 0.12          |
| (1,995)  | 1:A:69:VAL:HG11 | 1:A:72:ILE:HB   | 17       | 0.11          |
| (1,995)  | 1:A:69:VAL:HG12 | 1:A:72:ILE:HB   | 17       | 0.11          |
| (1,995)  | 1:A:69:VAL:HG13 | 1:A:72:ILE:HB   | 17       | 0.11          |
| (1,995)  | 1:A:69:VAL:HG21 | 1:A:72:ILE:HB   | 17       | 0.11          |
| (1,995)  | 1:A:69:VAL:HG22 | 1:A:72:ILE:HB   | 17       | 0.11          |
| (1,995)  | 1:A:69:VAL:HG23 | 1:A:72:ILE:HB   | 17       | 0.11          |
| (1,841)  | 1:A:35:ASP:HB2  | 1:A:36:GLY:HA3  | 15       | 0.11          |
| (1,841)  | 1:A:35:ASP:HB3  | 1:A:36:GLY:HA3  | 15       | 0.11          |
| (1,795)  | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD21 | 2        | 0.11          |
| (1,795)  | 1:A:16:TYR:HE1  | 1:A:82:ASN:HD22 | 2        | 0.11          |
| (1,795)  | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD21 | 2        | 0.11          |
| (1,795)  | 1:A:16:TYR:HE2  | 1:A:82:ASN:HD22 | 2        | 0.11          |
| (1,749)  | 1:A:68:LEU:HB2  | 1:A:73:LEU:HG   | 10       | 0.11          |
| (1,697)  | 1:A:31:PRO:HD2  | 1:A:45:ALA:HB1  | 14       | 0.11          |
| (1,697)  | 1:A:31:PRO:HD2  | 1:A:45:ALA:HB2  | 14       | 0.11          |
| (1,697)  | 1:A:31:PRO:HD2  | 1:A:45:ALA:HB3  | 14       | 0.11          |
| (1,697)  | 1:A:31:PRO:HD3  | 1:A:45:ALA:HB1  | 14       | 0.11          |
| (1,697)  | 1:A:31:PRO:HD3  | 1:A:45:ALA:HB2  | 14       | 0.11          |
| (1,697)  | 1:A:31:PRO:HD3  | 1:A:45:ALA:HB3  | 14       | 0.11          |
| (1,675)  | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 13       | 0.11          |
| (1,675)  | 1:A:76:PRO:HG2  | 1:A:79:GLY:HA3  | 17       | 0.11          |
| (1,569)  | 1:A:52:GLY:HA3  | 1:A:88:ASN:H    | 18       | 0.11          |
| (1,556)  | 1:A:40:LEU:HB3  | 1:A:41:SER:HA   | 20       | 0.11          |
| (1,468)  | 1:A:72:ILE:H    | 1:A:72:ILE:HG12 | 18       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,439)  | 1:A:39:LEU:H   | 1:A:39:LEU:HG   | 6        | 0.11          |
| (1,391)  | 1:A:33:GLU:H   | 1:A:38:VAL:HG11 | 7        | 0.11          |
| (1,391)  | 1:A:33:GLU:H   | 1:A:38:VAL:HG12 | 7        | 0.11          |
| (1,391)  | 1:A:33:GLU:H   | 1:A:38:VAL:HG13 | 7        | 0.11          |
| (1,353)  | 1:A:17:ILE:HB  | 1:A:75:ALA:HB1  | 19       | 0.11          |
| (1,353)  | 1:A:17:ILE:HB  | 1:A:75:ALA:HB2  | 19       | 0.11          |
| (1,353)  | 1:A:17:ILE:HB  | 1:A:75:ALA:HB3  | 19       | 0.11          |
| (1,311)  | 1:A:40:LEU:HB3 | 1:A:43:VAL:HB   | 20       | 0.11          |
| (1,234)  | 1:A:44:THR:HA  | 1:A:50:ALA:HB1  | 9        | 0.11          |
| (1,234)  | 1:A:44:THR:HA  | 1:A:50:ALA:HB2  | 9        | 0.11          |
| (1,234)  | 1:A:44:THR:HA  | 1:A:50:ALA:HB3  | 9        | 0.11          |
| (1,163)  | 1:A:21:GLU:HB3 | 1:A:85:TYR:HE1  | 8        | 0.11          |
| (1,163)  | 1:A:21:GLU:HB3 | 1:A:85:TYR:HE2  | 8        | 0.11          |
| (1,156)  | 1:A:46:GLN:HG3 | 1:A:47:PHE:HE1  | 2        | 0.11          |
| (1,156)  | 1:A:46:GLN:HG3 | 1:A:47:PHE:HE2  | 2        | 0.11          |
| (1,155)  | 1:A:67:ARG:HE  | 1:A:69:VAL:HB   | 7        | 0.11          |
| (1,104)  | 1:A:39:LEU:H   | 1:A:72:ILE:HA   | 16       | 0.11          |
| (1,1019) | 1:A:87:VAL:HA  | 1:A:88:ASN:HB2  | 5        | 0.11          |
| (1,1019) | 1:A:87:VAL:HA  | 1:A:88:ASN:HB3  | 5        | 0.11          |
| (1,1011) | 1:A:83:LEU:HA  | 1:A:84:VAL:HG11 | 20       | 0.11          |
| (1,1011) | 1:A:83:LEU:HA  | 1:A:84:VAL:HG12 | 20       | 0.11          |
| (1,1011) | 1:A:83:LEU:HA  | 1:A:84:VAL:HG13 | 20       | 0.11          |
| (1,1011) | 1:A:83:LEU:HA  | 1:A:84:VAL:HG21 | 20       | 0.11          |
| (1,1011) | 1:A:83:LEU:HA  | 1:A:84:VAL:HG22 | 20       | 0.11          |
| (1,1011) | 1:A:83:LEU:HA  | 1:A:84:VAL:HG23 | 20       | 0.11          |

## 10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value