



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 02:28 AM UTC

PDB ID : 2LJ0 / pdb\_00002lj0  
BMRB ID : 17912  
Title : The third SH3 domain of R85FL  
Authors : Jiang, Y.; Hu, H.  
Deposited on : 2011-09-02

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)

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

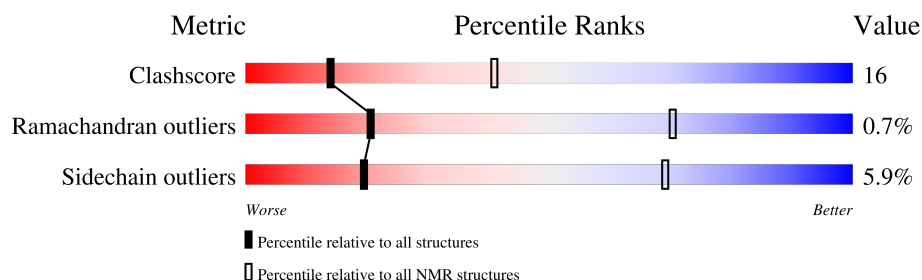
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 65     |                  |

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 12 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:7-A:63 (57)         | 0.39              | 12           |

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                     | 1, 3, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15 |
| 2                     | 2, 5                                     |
| Single-model clusters | 4                                        |

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

There is only 1 type of molecule in this entry. The entry contains 1035 atoms, of which 500 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sorbin and SH3 domain-containing protein 1.

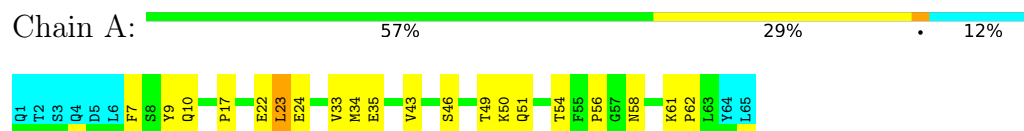
| Mol | Chain | Residues | Atoms |     |     |    |     |   | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|-------|
| 1   | A     | 65       | Total | C   | H   | N  | O   | S | 0     |
|     |       |          | 1035  | 340 | 500 | 85 | 108 | 2 |       |

## 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: Sorbin and SH3 domain-containing protein 1

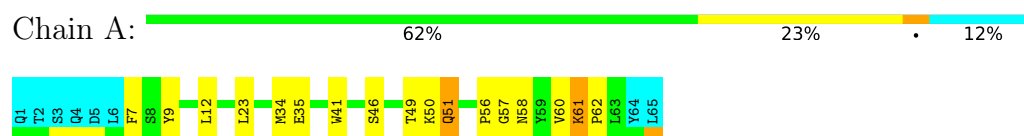


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

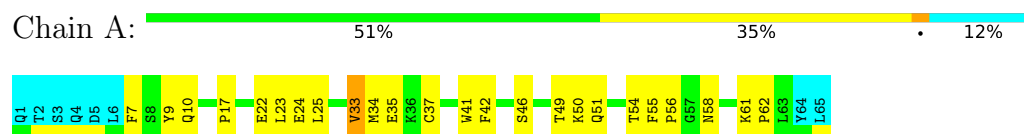
#### 4.2.1 Score per residue for model 1

- Molecule 1: Sorbin and SH3 domain-containing protein 1



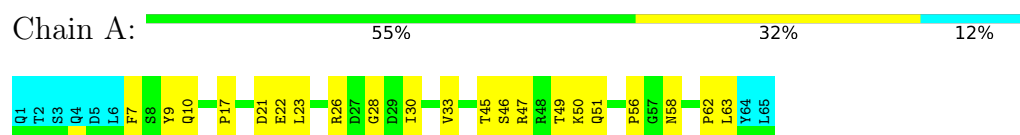
#### 4.2.2 Score per residue for model 2

- Molecule 1: Sorbin and SH3 domain-containing protein 1



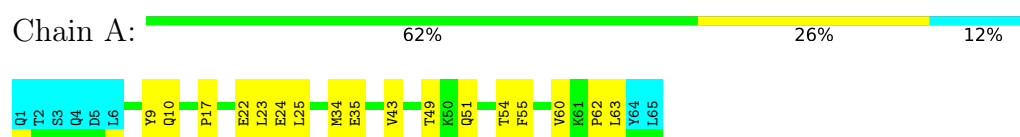
### 4.2.3 Score per residue for model 3

- Molecule 1: Sorbin and SH3 domain-containing protein 1



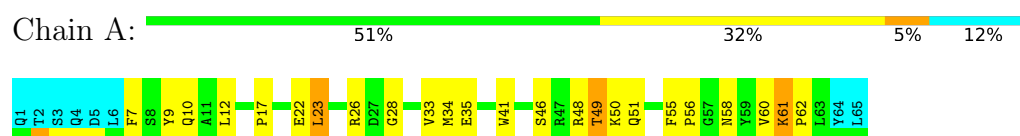
### 4.2.4 Score per residue for model 4

- Molecule 1: Sorbin and SH3 domain-containing protein 1



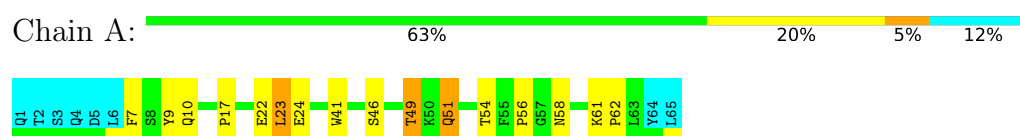
### 4.2.5 Score per residue for model 5

- Molecule 1: Sorbin and SH3 domain-containing protein 1



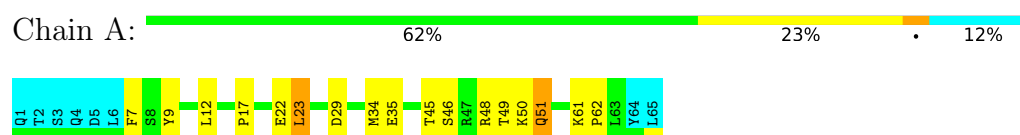
### 4.2.6 Score per residue for model 6

- Molecule 1: Sorbin and SH3 domain-containing protein 1



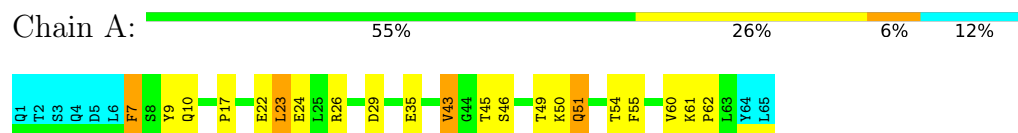
### 4.2.7 Score per residue for model 7

- Molecule 1: Sorbin and SH3 domain-containing protein 1



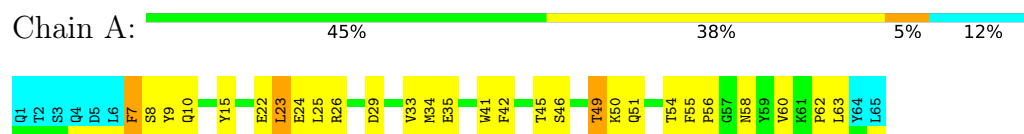
### 4.2.8 Score per residue for model 8

- Molecule 1: Sorbin and SH3 domain-containing protein 1



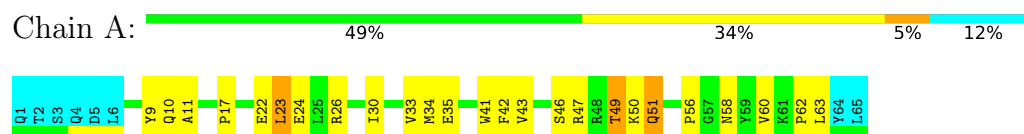
### 4.2.9 Score per residue for model 9

- Molecule 1: Sorbin and SH3 domain-containing protein 1



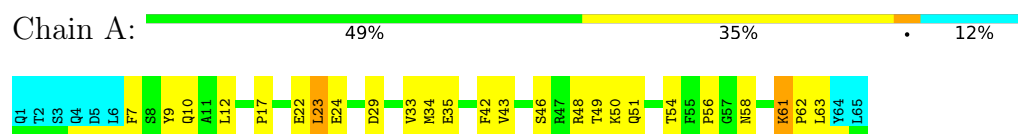
### 4.2.10 Score per residue for model 10

- Molecule 1: Sorbin and SH3 domain-containing protein 1



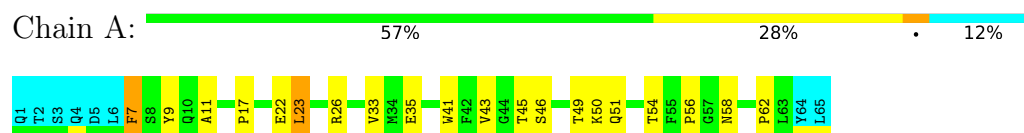
### 4.2.11 Score per residue for model 11

- Molecule 1: Sorbin and SH3 domain-containing protein 1



### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Sorbin and SH3 domain-containing protein 1





## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| ARIA          | structure solution |         |
| ARIA          | 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                       | 706            |
| Number of shifts mapped to atoms             | 706            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 81%            |

## 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     | 467   | 435      | 435      | 14±2    |
| All | All   | 7005  | 6525     | 6525     | 213     |

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 16.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:23:LEU:HD11 | 1:A:46:SER:HB2  | 0.78     | 1.54        | 14     | 14    |
| 1:A:17:PRO:HB3  | 1:A:22:GLU:HB2  | 0.77     | 1.54        | 12     | 13    |
| 1:A:22:GLU:HG2  | 1:A:54:THR:HG23 | 0.72     | 1.60        | 11     | 5     |
| 1:A:23:LEU:HD21 | 1:A:51:GLN:HG3  | 0.72     | 1.61        | 4      | 12    |
| 1:A:35:GLU:HB3  | 1:A:43:VAL:HB   | 0.70     | 1.62        | 4      | 5     |
| 1:A:12:LEU:HD21 | 1:A:61:LYS:HE2  | 0.67     | 1.65        | 5      | 3     |
| 1:A:10:GLN:HB2  | 1:A:63:LEU:HD11 | 0.67     | 1.65        | 11     | 7     |
| 1:A:12:LEU:HD21 | 1:A:61:LYS:HE3  | 0.66     | 1.67        | 7      | 1     |
| 1:A:26:ARG:HG3  | 1:A:29:ASP:HB2  | 0.65     | 1.68        | 8      | 2     |
| 1:A:18:GLN:HE21 | 1:A:18:GLN:HA   | 0.65     | 1.51        | 15     | 1     |
| 1:A:9:TYR:HD1   | 1:A:62:PRO:HA   | 0.61     | 1.55        | 7      | 14    |
| 1:A:49:THR:HG23 | 1:A:51:GLN:HG2  | 0.58     | 1.76        | 6      | 5     |
| 1:A:9:TYR:CD1   | 1:A:62:PRO:HA   | 0.57     | 2.35        | 2      | 14    |
| 1:A:10:GLN:O    | 1:A:61:LYS:HG2  | 0.57     | 1.99        | 14     | 5     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:9:TYR:HB3   | 1:A:60:VAL:HB   | 0.54     | 1.78        | 10     | 6     |
| 1:A:41:TRP:HZ3  | 1:A:58:ASN:HB2  | 0.53     | 1.63        | 5      | 7     |
| 1:A:34:MET:HG3  | 1:A:35:GLU:N    | 0.52     | 2.19        | 11     | 7     |
| 1:A:25:LEU:HD21 | 1:A:55:PHE:HB2  | 0.52     | 1.82        | 4      | 2     |
| 1:A:55:PHE:HE2  | 1:A:60:VAL:HG21 | 0.51     | 1.66        | 4      | 3     |
| 1:A:23:LEU:CD2  | 1:A:51:GLN:HG3  | 0.50     | 2.36        | 2      | 4     |
| 1:A:12:LEU:CD2  | 1:A:61:LYS:HE2  | 0.49     | 2.36        | 1      | 1     |
| 1:A:49:THR:HG21 | 1:A:51:GLN:HE21 | 0.49     | 1.67        | 5      | 1     |
| 1:A:46:SER:O    | 1:A:50:LYS:HA   | 0.49     | 2.07        | 5      | 13    |
| 1:A:33:VAL:HG21 | 1:A:42:PHE:HB3  | 0.49     | 1.84        | 2      | 2     |
| 1:A:30:ILE:CG2  | 1:A:47:ARG:HD2  | 0.48     | 2.39        | 3      | 2     |
| 1:A:33:VAL:CG2  | 1:A:42:PHE:HB3  | 0.47     | 2.38        | 10     | 5     |
| 1:A:10:GLN:HG2  | 1:A:61:LYS:NZ   | 0.47     | 2.25        | 13     | 1     |
| 1:A:17:PRO:HB3  | 1:A:22:GLU:CB   | 0.46     | 2.39        | 15     | 4     |
| 1:A:10:GLN:HE21 | 1:A:28:GLY:HA2  | 0.46     | 1.71        | 5      | 2     |
| 1:A:23:LEU:HD13 | 1:A:24:GLU:N    | 0.46     | 2.26        | 13     | 10    |
| 1:A:7:PHE:HB3   | 1:A:33:VAL:HG13 | 0.45     | 1.87        | 3      | 2     |
| 1:A:26:ARG:HD3  | 1:A:48:ARG:HH12 | 0.45     | 1.72        | 13     | 1     |
| 1:A:56:PRO:C    | 1:A:58:ASN:H    | 0.45     | 2.19        | 6      | 11    |
| 1:A:37:CYS:HB2  | 1:A:41:TRP:O    | 0.45     | 2.11        | 2      | 1     |
| 1:A:22:GLU:HA   | 1:A:54:THR:O    | 0.45     | 2.12        | 15     | 5     |
| 1:A:29:ASP:OD1  | 1:A:48:ARG:HB2  | 0.44     | 2.11        | 11     | 2     |
| 1:A:45:THR:HA   | 1:A:51:GLN:O    | 0.44     | 2.13        | 9      | 6     |
| 1:A:23:LEU:HB3  | 1:A:55:PHE:HB3  | 0.43     | 1.91        | 9      | 1     |
| 1:A:9:TYR:CE2   | 1:A:33:VAL:HG11 | 0.42     | 2.49        | 12     | 1     |
| 1:A:11:ALA:HB3  | 1:A:26:ARG:O    | 0.42     | 2.14        | 10     | 2     |
| 1:A:34:MET:SD   | 1:A:35:GLU:N    | 0.42     | 2.92        | 7      | 2     |
| 1:A:9:TYR:CB    | 1:A:60:VAL:HB   | 0.41     | 2.45        | 10     | 1     |
| 1:A:26:ARG:CG   | 1:A:29:ASP:HB2  | 0.41     | 2.41        | 9      | 1     |
| 1:A:56:PRO:HB2  | 1:A:59:TYR:CD2  | 0.41     | 2.50        | 14     | 1     |
| 1:A:31:VAL:HG22 | 1:A:46:SER:HA   | 0.41     | 1.92        | 14     | 1     |
| 1:A:15:TYR:HB3  | 1:A:25:LEU:HB2  | 0.40     | 1.92        | 9      | 1     |
| 1:A:26:ARG:HD2  | 1:A:48:ARG:NH1  | 0.40     | 2.31        | 5      | 1     |
| 1:A:57:GLY:HA2  | 1:A:60:VAL:HG22 | 0.40     | 1.92        | 1      | 1     |
| 1:A:34:MET:CG   | 1:A:43:VAL:HG12 | 0.40     | 2.47        | 13     | 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     | 57/65 (88%)   | 53±1 (93±2%) | 4±1 (6±2%) | 0±1 (1±1%) | 20          | 70 |
| All | All   | 855/975 (88%) | 796 (93%)    | 53 (6%)    | 6 (1%)     | 20          | 70 |

All 3 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     | 7   | PHE  | 4              |
| 1   | A     | 21  | ASP  | 1              |
| 1   | A     | 27  | ASP  | 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     | 51/59 (86%)   | 48±1 (94±2%) | 3±1 (6±2%) | 19          | 69 |
| All | All   | 765/885 (86%) | 720 (94%)    | 45 (6%)    | 19          | 69 |

All 9 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     | 49  | THR  | 13             |
| 1   | A     | 23  | LEU  | 11             |
| 1   | A     | 51  | GLN  | 7              |
| 1   | A     | 7   | PHE  | 5              |
| 1   | A     | 61  | LYS  | 3              |
| 1   | A     | 33  | VAL  | 2              |
| 1   | A     | 43  | VAL  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 26  | ARG  | 1              |
| 1   | A     | 18  | GLN  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 79% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 706 |
| Number of shifts mapped to atoms        | 706 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 21  |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 64       | $-0.24 \pm 0.26$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 59       | $-0.13 \pm 0.18$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 59       | $-0.08 \pm 0.23$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 62       | $-0.34 \pm 0.50$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 626 atoms were assigned a chemical shift out of a possible 774. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 281/284 (99%) | 116/116 (100%) | 111/114 (97%)   | 54/54 (100%)    |
| Sidechain | 328/402 (82%) | 221/257 (86%)  | 103/128 (80%)   | 4/17 (24%)      |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 17/88 (19%)   | 17/42 (40%)    | 0/45 (0%)       | 0/1 (0%)        |
| Overall  | 626/774 (81%) | 354/415 (85%)  | 214/287 (75%)   | 58/72 (81%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 702 atoms were assigned a chemical shift out of a possible 885. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 316/324 (98%) | 131/132 (99%)  | 123/130 (95%)   | 62/62 (100%)    |
| Sidechain | 367/464 (79%) | 246/297 (83%)  | 117/148 (79%)   | 4/19 (21%)      |
| Aromatic  | 19/97 (20%)   | 19/46 (41%)    | 0/50 (0%)       | 0/1 (0%)        |
| Overall   | 702/885 (79%) | 396/475 (83%)  | 240/328 (73%)   | 66/82 (80%)     |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

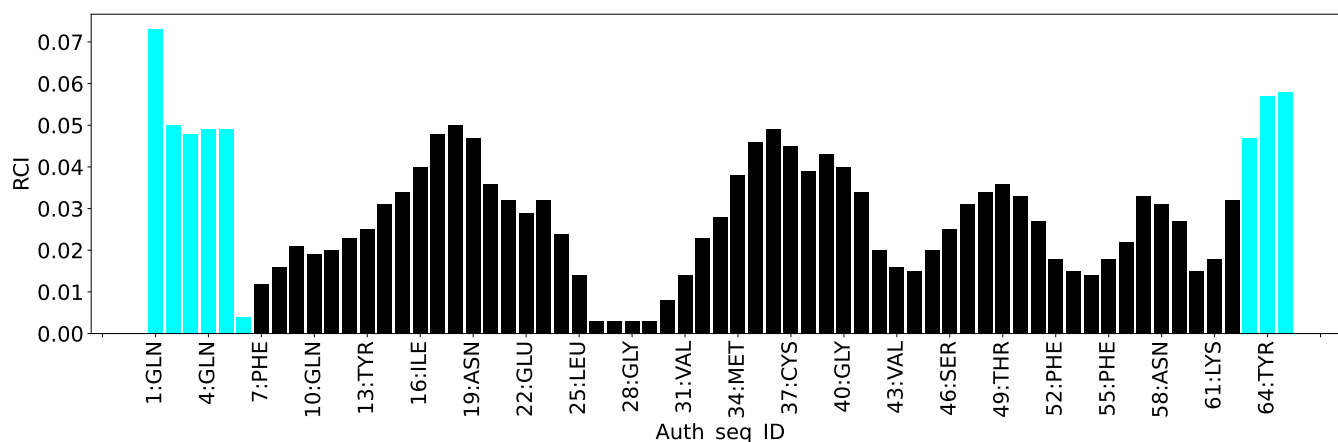
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 2   | THR  | CB   | 0.00       | 61.12 – 78.27       | -40.6   |
| 1       | A     | 29  | ASP  | CA   | 0.00       | 44.71 – 64.67       | -27.4   |
| 1       | A     | 6   | LEU  | CA   | 0.00       | 45.17 – 66.21       | -26.5   |
| 1       | A     | 65  | LEU  | CA   | 0.00       | 45.17 – 66.21       | -26.5   |
| 1       | A     | 26  | ARG  | CA   | 0.00       | 45.44 – 68.13       | -25.0   |
| 1       | A     | 65  | LEU  | CG   | 0.00       | 21.37 – 32.19       | -24.8   |
| 1       | A     | 2   | THR  | CA   | 0.00       | 49.41 – 75.05       | -24.3   |
| 1       | A     | 64  | TYR  | CA   | 0.00       | 45.75 – 70.63       | -23.4   |
| 1       | A     | 49  | THR  | HG1  | 5.79       | 0.08 – 2.19         | 22.0    |
| 1       | A     | 45  | THR  | HG1  | 5.68       | 0.08 – 2.19         | 21.6    |
| 1       | A     | 54  | THR  | HG1  | 5.30       | 0.08 – 2.19         | 19.7    |
| 1       | A     | 6   | LEU  | CD1  | 0.00       | 16.71 – 32.55       | -15.6   |
| 1       | A     | 65  | LEU  | CD1  | 0.00       | 16.71 – 32.55       | -15.6   |
| 1       | A     | 65  | LEU  | CD2  | 0.00       | 15.73 – 32.47       | -14.4   |
| 1       | A     | 2   | THR  | HB   | 0.00       | 2.57 – 5.77         | -13.0   |
| 1       | A     | 56  | PRO  | HG3  | 0.18       | 0.33 – 3.48         | -5.5    |
| 1       | A     | 36  | LYS  | HG3  | -0.07      | 0.04 – 2.67         | -5.4    |
| 1       | A     | 2   | THR  | HG21 | 0.00       | 0.08 – 2.19         | -5.4    |
| 1       | A     | 2   | THR  | HG22 | 0.00       | 0.08 – 2.19         | -5.4    |
| 1       | A     | 2   | THR  | HG23 | 0.00       | 0.08 – 2.19         | -5.4    |
| 1       | A     | 56  | PRO  | HD2  | 1.85       | 1.93 – 5.38         | -5.2    |

### 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                                | 1168  |
| Intra-residue ( $ i-j =0$ )                              | 513   |
| Sequential ( $ i-j =1$ )                                 | 280   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 55    |
| Long range ( $ i-j \geq 5$ )                             | 320   |
| 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                         | 18.0  |
| Number of long range restraints per residue <sup>1</sup> | 4.9   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 25.7                                   | 0.2     |
| 0.2-0.5 (Medium) | 39.3                                   | 0.5     |
| >0.5 (Large)     | 91.8                                   | 4.14    |

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

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

## 9 Distance violation analysis ⓘ

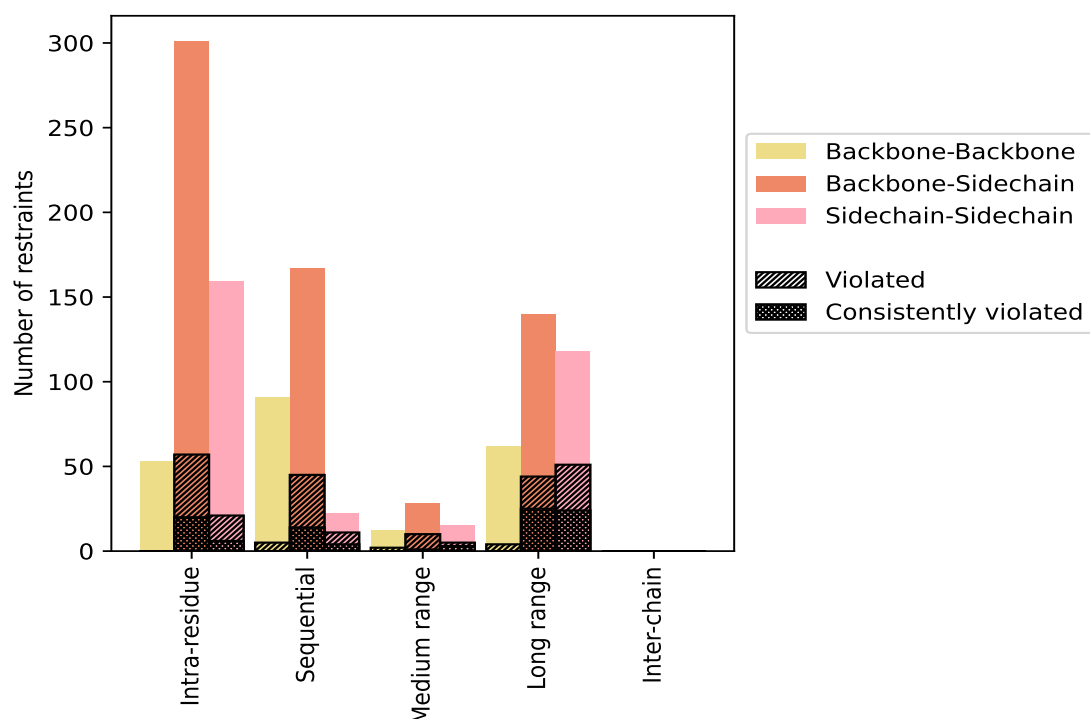
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count                | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                     |
|------------------------------------------------------------|----------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|---------------------|
|                                                            |                      |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">513</a>  | <a href="#">43.9</a>  | <a href="#">78</a>    | <a href="#">15.2</a> | <a href="#">6.7</a>  | <a href="#">26</a>                 | <a href="#">5.1</a>  | <a href="#">2.2</a> |
| Backbone-Backbone                                          | 53                   | 4.5                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 301                  | 25.8                  | 57                    | 18.9                 | 4.9                  | 20                                 | 6.6                  | 1.7                 |
| Sidechain-Sidechain                                        | 159                  | 13.6                  | 21                    | 13.2                 | 1.8                  | 6                                  | 3.8                  | 0.5                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">280</a>  | <a href="#">24.0</a>  | <a href="#">61</a>    | <a href="#">21.8</a> | <a href="#">5.2</a>  | <a href="#">18</a>                 | <a href="#">6.4</a>  | <a href="#">1.5</a> |
| Backbone-Backbone                                          | 91                   | 7.8                   | 5                     | 5.5                  | 0.4                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 167                  | 14.3                  | 45                    | 26.9                 | 3.9                  | 14                                 | 8.4                  | 1.2                 |
| Sidechain-Sidechain                                        | 22                   | 1.9                   | 11                    | 50.0                 | 0.9                  | 4                                  | 18.2                 | 0.3                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">55</a>   | <a href="#">4.7</a>   | <a href="#">17</a>    | <a href="#">30.9</a> | <a href="#">1.5</a>  | <a href="#">4</a>                  | <a href="#">7.3</a>  | <a href="#">0.3</a> |
| Backbone-Backbone                                          | 12                   | 1.0                   | 2                     | 16.7                 | 0.2                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 28                   | 2.4                   | 10                    | 35.7                 | 0.9                  | 1                                  | 3.6                  | 0.1                 |
| Sidechain-Sidechain                                        | 15                   | 1.3                   | 5                     | 33.3                 | 0.4                  | 3                                  | 20.0                 | 0.3                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">320</a>  | <a href="#">27.4</a>  | <a href="#">99</a>    | <a href="#">30.9</a> | <a href="#">8.5</a>  | <a href="#">49</a>                 | <a href="#">15.3</a> | <a href="#">4.2</a> |
| Backbone-Backbone                                          | 62                   | 5.3                   | 4                     | 6.5                  | 0.3                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 140                  | 12.0                  | 44                    | 31.4                 | 3.8                  | 25                                 | 17.9                 | 2.1                 |
| Sidechain-Sidechain                                        | 118                  | 10.1                  | 51                    | 43.2                 | 4.4                  | 24                                 | 20.3                 | 2.1                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">1168</a> | <a href="#">100.0</a> | <a href="#">255</a>   | <a href="#">21.8</a> | <a href="#">21.8</a> | <a href="#">97</a>                 | <a href="#">8.3</a>  | <a href="#">8.3</a> |
| Backbone-Backbone                                          | 218                  | 18.7                  | 11                    | 5.0                  | 0.9                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 636                  | 54.5                  | 156                   | 24.5                 | 13.4                 | 60                                 | 9.4                  | 5.1                 |
| Sidechain-Sidechain                                        | 314                  | 26.9                  | 88                    | 28.0                 | 7.5                  | 37                                 | 11.8                 | 3.2                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 38                   | 32              | 10              | 76              | 0               | 156   | 0.84     | 4.06    | 0.75                | 0.61       |
| 2        | 44                   | 36              | 7               | 74              | 0               | 161   | 0.84     | 3.98    | 0.77                | 0.58       |
| 3        | 41                   | 35              | 7               | 74              | 0               | 157   | 0.83     | 4.03    | 0.74                | 0.61       |
| 4        | 47                   | 35              | 11              | 66              | 0               | 159   | 0.85     | 4.04    | 0.77                | 0.59       |
| 5        | 47                   | 32              | 7               | 74              | 0               | 160   | 0.82     | 4.04    | 0.74                | 0.58       |
| 6        | 45                   | 33              | 7               | 79              | 0               | 164   | 0.81     | 4.14    | 0.74                | 0.59       |
| 7        | 40                   | 40              | 7               | 72              | 0               | 159   | 0.86     | 3.88    | 0.75                | 0.68       |
| 8        | 46                   | 37              | 9               | 72              | 0               | 164   | 0.87     | 4.09    | 0.77                | 0.66       |
| 9        | 44                   | 35              | 9               | 72              | 0               | 160   | 0.9      | 3.74    | 0.77                | 0.7        |
| 10       | 46                   | 34              | 8               | 70              | 0               | 158   | 0.87     | 3.93    | 0.76                | 0.66       |

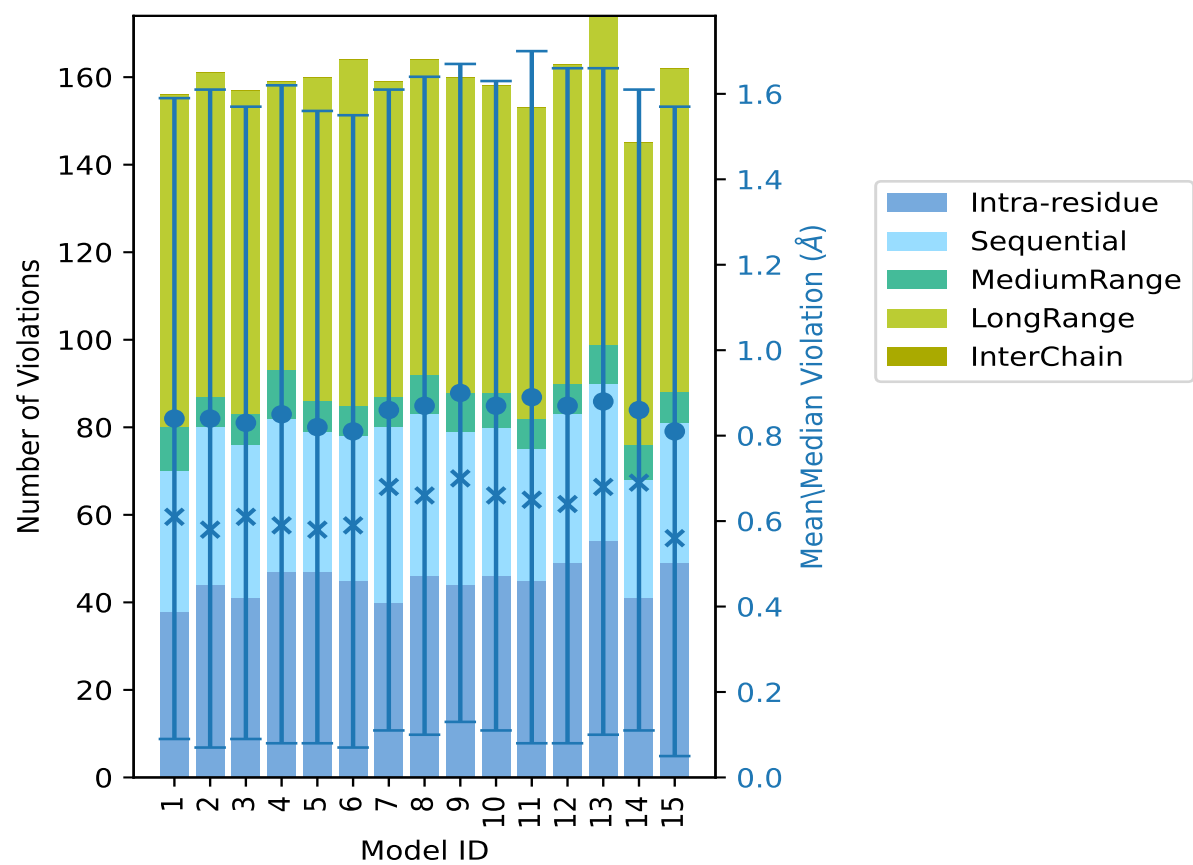
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 45                   | 30              | 7               | 71              | 0               | 153   | 0.89     | 4.09    | 0.81                | 0.65       |
| 12       | 49                   | 34              | 7               | 73              | 0               | 163   | 0.87     | 4.04    | 0.79                | 0.64       |
| 13       | 54                   | 36              | 9               | 75              | 0               | 174   | 0.88     | 4.06    | 0.78                | 0.68       |
| 14       | 41                   | 27              | 8               | 69              | 0               | 145   | 0.86     | 3.95    | 0.75                | 0.69       |
| 15       | 49                   | 32              | 7               | 74              | 0               | 162   | 0.81     | 4.11    | 0.76                | 0.56       |

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

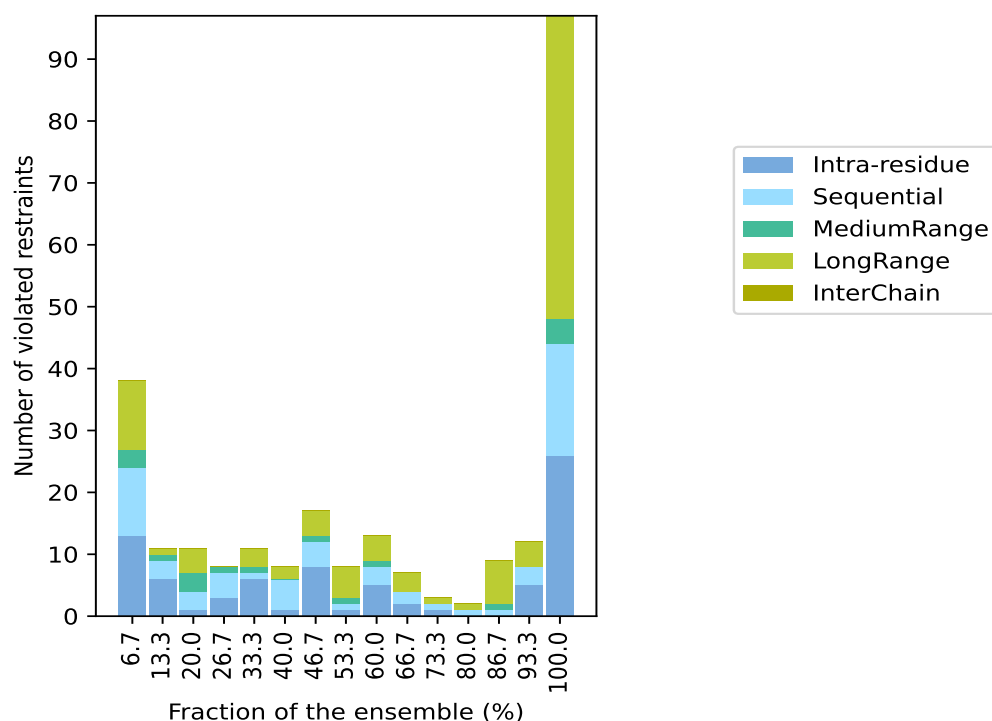
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 913(IR:435, SQ:219, MR:38, LR:221, IC:0) restraints are not 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>       | %     |
| 13                            | 11              | 3               | 11              | 0               | 38    | 1                        | 6.7   |
| 6                             | 3               | 1               | 1               | 0               | 11    | 2                        | 13.3  |
| 1                             | 3               | 3               | 4               | 0               | 11    | 3                        | 20.0  |
| 3                             | 4               | 1               | 0               | 0               | 8     | 4                        | 26.7  |
| 6                             | 1               | 1               | 3               | 0               | 11    | 5                        | 33.3  |
| 1                             | 5               | 0               | 2               | 0               | 8     | 6                        | 40.0  |
| 8                             | 4               | 1               | 4               | 0               | 17    | 7                        | 46.7  |
| 1                             | 1               | 1               | 5               | 0               | 8     | 8                        | 53.3  |
| 5                             | 3               | 1               | 4               | 0               | 13    | 9                        | 60.0  |
| 2                             | 2               | 0               | 3               | 0               | 7     | 10                       | 66.7  |
| 1                             | 1               | 0               | 1               | 0               | 3     | 11                       | 73.3  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 12                       | 80.0  |
| 0                             | 1               | 1               | 7               | 0               | 9     | 13                       | 86.7  |
| 5                             | 3               | 0               | 4               | 0               | 12    | 14                       | 93.3  |
| 26                            | 18              | 4               | 49              | 0               | 97    | 15                       | 100.0 |

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

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

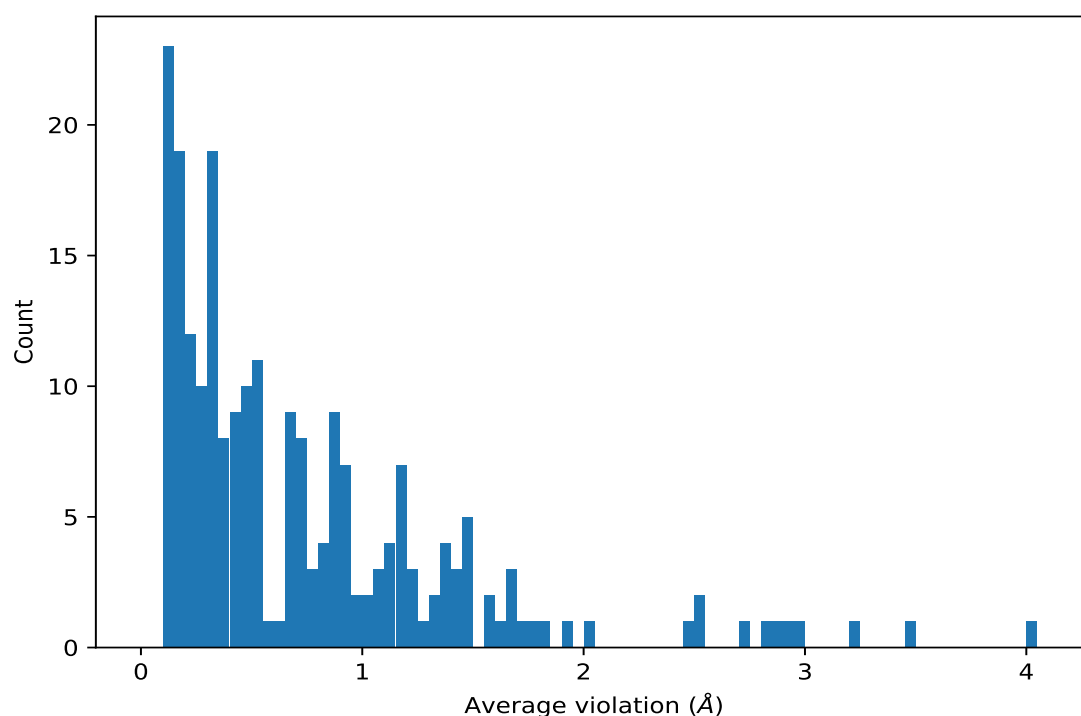
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,882)  | 1:45:A:THR:H    | 1:52:A:PHE:HD2  | 15                  | 4.01     | 0.1                 | 4.04       |
| (1,625)  | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1   | 15                  | 3.47     | 0.12                | 3.48       |
| (1,624)  | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1   | 15                  | 3.21     | 0.18                | 3.19       |
| (1,113)  | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2  | 15                  | 2.96     | 0.14                | 2.99       |
| (1,645)  | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1   | 15                  | 2.88     | 0.06                | 2.89       |
| (1,546)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2  | 15                  | 2.82     | 0.13                | 2.8        |
| (1,118)  | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2  | 15                  | 2.73     | 0.1                 | 2.76       |
| (1,516)  | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1   | 15                  | 2.54     | 0.22                | 2.5        |
| (1,515)  | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1   | 15                  | 2.52     | 0.19                | 2.5        |
| (1,470)  | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1  | 15                  | 2.45     | 0.13                | 2.47       |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 15                  | 1.92     | 0.12                | 1.96       |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 15                  | 1.81     | 0.54                | 1.5        |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 15                  | 1.76     | 0.05                | 1.76       |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 15                  | 1.69     | 0.72                | 1.25       |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 15                  | 1.67     | 0.35                | 1.78       |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 15                  | 1.67     | 0.09                | 1.71       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 15                  | 1.64     | 0.04                | 1.64       |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 15                  | 1.59     | 0.08                | 1.58       |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 15                  | 1.55     | 0.1                 | 1.57       |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 15                  | 1.47     | 0.07                | 1.49       |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 15                  | 1.47     | 0.05                | 1.48       |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 15                  | 1.46     | 0.06                | 1.47       |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 15                  | 1.45     | 0.07                | 1.46       |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 15                  | 1.45     | 0.07                | 1.44       |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 15                  | 1.42     | 0.1                 | 1.48       |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 15                  | 1.41     | 0.18                | 1.4        |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 15                  | 1.4      | 0.04                | 1.41       |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 15                  | 1.39     | 0.09                | 1.39       |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 15                  | 1.39     | 0.06                | 1.4        |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 15                  | 1.33     | 0.41                | 1.53       |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 15                  | 1.24     | 0.01                | 1.24       |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 15                  | 1.23     | 0.03                | 1.23       |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 15                  | 1.2      | 0.5                 | 1.52       |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 15                  | 1.19     | 0.08                | 1.17       |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 15                  | 1.18     | 0.18                | 1.26       |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 15                  | 1.18     | 0.41                | 1.1        |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 15                  | 1.15     | 0.2                 | 1.18       |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 15                  | 1.15     | 0.08                | 1.16       |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 15                  | 1.09     | 0.02                | 1.09       |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 15                  | 1.06     | 0.11                | 1.05       |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 15                  | 1.01     | 0.13                | 1.0        |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 15                  | 1.0      | 0.14                | 1.05       |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 15                  | 0.98     | 0.02                | 0.98       |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 15                  | 0.93     | 0.07                | 0.95       |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 15                  | 0.92     | 0.23                | 0.97       |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 15                  | 0.92     | 0.07                | 0.94       |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 15                  | 0.92     | 0.16                | 0.92       |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 15                  | 0.91     | 0.11                | 0.91       |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 15                  | 0.9      | 0.11                | 0.87       |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 15                  | 0.9      | 0.11                | 0.88       |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 15                  | 0.87     | 0.28                | 0.92       |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 15                  | 0.87     | 0.07                | 0.86       |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 15                  | 0.87     | 0.14                | 0.87       |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 15                  | 0.85     | 0.38                | 0.81       |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 15                  | 0.85     | 0.14                | 0.88       |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 15                  | 0.84     | 0.04                | 0.86       |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 15                  | 0.81     | 0.14                | 0.8        |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 15                  | 0.81     | 0.05                | 0.81       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 15                  | 0.74     | 0.14                | 0.73       |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 15                  | 0.74     | 0.06                | 0.72       |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 15                  | 0.71     | 0.03                | 0.71       |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 15                  | 0.71     | 0.14                | 0.64       |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 15                  | 0.7      | 0.11                | 0.69       |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 15                  | 0.68     | 0.11                | 0.66       |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 15                  | 0.68     | 0.09                | 0.65       |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 15                  | 0.66     | 0.04                | 0.67       |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 15                  | 0.66     | 0.05                | 0.66       |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 15                  | 0.65     | 0.06                | 0.67       |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 15                  | 0.65     | 0.08                | 0.62       |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 15                  | 0.65     | 0.13                | 0.66       |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 15                  | 0.52     | 0.03                | 0.53       |
| (1,372)  | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 15                  | 0.52     | 0.0                 | 0.52       |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 15                  | 0.51     | 0.01                | 0.51       |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 15                  | 0.5      | 0.02                | 0.5        |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 15                  | 0.49     | 0.0                 | 0.49       |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 15                  | 0.49     | 0.14                | 0.57       |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 15                  | 0.47     | 0.08                | 0.48       |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 15                  | 0.46     | 0.01                | 0.47       |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 15                  | 0.44     | 0.22                | 0.49       |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 15                  | 0.41     | 0.06                | 0.4        |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 15                  | 0.41     | 0.03                | 0.42       |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 15                  | 0.4      | 0.0                 | 0.4        |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 15                  | 0.36     | 0.07                | 0.38       |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 15                  | 0.35     | 0.06                | 0.35       |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 15                  | 0.34     | 0.04                | 0.34       |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 15                  | 0.32     | 0.04                | 0.33       |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 15                  | 0.31     | 0.11                | 0.29       |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 15                  | 0.3      | 0.07                | 0.3        |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 15                  | 0.27     | 0.01                | 0.27       |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 15                  | 0.25     | 0.03                | 0.26       |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 15                  | 0.23     | 0.0                 | 0.23       |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 15                  | 0.23     | 0.05                | 0.23       |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 15                  | 0.22     | 0.03                | 0.22       |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 15                  | 0.2      | 0.01                | 0.2        |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 15                  | 0.2      | 0.04                | 0.2        |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 15                  | 0.17     | 0.02                | 0.16       |
| (1,97)   | 1:42:A:PHE:HA   | 1:42:A:PHE:HB2  | 15                  | 0.15     | 0.0                 | 0.15       |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 14                  | 1.1      | 0.51                | 1.04       |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 14                  | 0.72     | 0.31                | 0.72       |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 14                  | 0.46     | 0.35                | 0.4        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 14                  | 0.39     | 0.11                | 0.4        |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 14                  | 0.39     | 0.62                | 0.13       |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 14                  | 0.33     | 0.05                | 0.35       |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 14                  | 0.33     | 0.16                | 0.27       |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 14                  | 0.29     | 0.13                | 0.3        |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 14                  | 0.19     | 0.01                | 0.19       |
| (1,785)  | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 14                  | 0.16     | 0.05                | 0.15       |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 14                  | 0.15     | 0.02                | 0.16       |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 14                  | 0.11     | 0.0                 | 0.11       |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 13                  | 1.38     | 0.57                | 1.38       |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 13                  | 1.13     | 0.65                | 1.05       |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 13                  | 0.89     | 0.51                | 1.13       |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 13                  | 0.47     | 0.33                | 0.34       |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 13                  | 0.42     | 0.15                | 0.4        |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 13                  | 0.39     | 0.17                | 0.34       |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 13                  | 0.34     | 0.08                | 0.37       |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 13                  | 0.32     | 0.06                | 0.32       |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 13                  | 0.3      | 0.09                | 0.34       |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 12                  | 1.19     | 0.65                | 1.51       |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 12                  | 0.17     | 0.03                | 0.17       |
| (1,84)   | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 11                  | 0.52     | 0.0                 | 0.52       |
| (1,405)  | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 11                  | 0.2      | 0.22                | 0.13       |
| (1,1112) | 1:55:A:PHE:H    | 1:42:A:PHE:HB3  | 11                  | 0.18     | 0.04                | 0.18       |
| (1,329)  | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1  | 10                  | 2.94     | 0.96                | 3.22       |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 10                  | 0.37     | 0.13                | 0.43       |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 10                  | 0.34     | 0.15                | 0.34       |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 10                  | 0.34     | 0.01                | 0.34       |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 10                  | 0.3      | 0.07                | 0.3        |
| (1,528)  | 1:35:A:GLU:HB2  | 1:36:A:LYS:H    | 10                  | 0.18     | 0.04                | 0.16       |
| (1,458)  | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 10                  | 0.12     | 0.02                | 0.11       |
| (1,321)  | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1  | 9                   | 2.02     | 0.14                | 2.03       |
| (1,320)  | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 9                   | 1.72     | 0.25                | 1.73       |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 9                   | 1.14     | 0.08                | 1.12       |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 9                   | 0.74     | 0.03                | 0.75       |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 9                   | 0.42     | 0.02                | 0.43       |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 9                   | 0.38     | 0.11                | 0.44       |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 9                   | 0.34     | 0.06                | 0.33       |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 9                   | 0.34     | 0.16                | 0.33       |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 9                   | 0.29     | 0.11                | 0.36       |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 9                   | 0.27     | 0.17                | 0.16       |
| (1,580)  | 1:50:A:LYS:HA   | 1:45:A:THR:HG21 | 9                   | 0.24     | 0.07                | 0.24       |
| (1,557)  | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 9                   | 0.13     | 0.02                | 0.13       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,330)  | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 9                   | 0.12     | 0.02                | 0.12       |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 8                   | 0.85     | 0.34                | 0.98       |
| (1,338)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 8                   | 0.82     | 0.54                | 1.1        |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 8                   | 0.69     | 0.36                | 0.56       |
| (1,538)  | 1:37:A:CYS:HB2  | 1:40:A:GLY:H    | 8                   | 0.33     | 0.51                | 0.14       |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 8                   | 0.19     | 0.07                | 0.16       |
| (1,994)  | 1:34:A:MET:H    | 1:44:A:GLY:HA3  | 8                   | 0.17     | 0.04                | 0.16       |
| (1,142)  | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 8                   | 0.15     | 0.04                | 0.15       |
| (1,568)  | 1:48:A:ARG:HB2  | 1:49:A:THR:HG23 | 8                   | 0.14     | 0.02                | 0.14       |
| (1,945)  | 1:26:A:ARG:H    | 1:25:A:LEU:HD22 | 7                   | 1.35     | 0.1                 | 1.37       |
| (1,1147) | 1:64:A:TYR:H    | 1:64:A:TYR:HD1  | 7                   | 1.11     | 0.4                 | 1.04       |
| (1,708)  | 1:8:A:SER:HB3   | 1:8:A:SER:H     | 7                   | 0.98     | 0.03                | 0.98       |
| (1,300)  | 1:10:A:GLN:HG2  | 1:61:A:LYS:HG3  | 7                   | 0.77     | 0.22                | 0.79       |
| (1,129)  | 1:45:A:THR:HB   | 1:32:A:ASP:HB2  | 7                   | 0.74     | 0.17                | 0.79       |
| (1,26)   | 1:25:A:LEU:HB2  | 1:25:A:LEU:HD22 | 7                   | 0.46     | 0.0                 | 0.46       |
| (1,471)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD22 | 7                   | 0.41     | 0.03                | 0.42       |
| (1,61)   | 1:34:A:MET:HB2  | 1:34:A:MET:HG2  | 7                   | 0.39     | 0.01                | 0.4        |
| (1,532)  | 1:36:A:LYS:HD2  | 1:36:A:LYS:HA   | 7                   | 0.31     | 0.08                | 0.34       |
| (1,274)  | 1:8:A:SER:HB2   | 1:63:A:LEU:HB3  | 7                   | 0.31     | 0.04                | 0.32       |
| (1,240)  | 1:3:A:SER:HA    | 1:3:A:SER:HB2   | 7                   | 0.21     | 0.0                 | 0.21       |
| (1,679)  | 1:33:A:VAL:H    | 1:32:A:ASP:HB2  | 7                   | 0.19     | 0.05                | 0.19       |
| (1,356)  | 1:52:A:PHE:HA   | 1:45:A:THR:HG21 | 7                   | 0.17     | 0.03                | 0.17       |
| (1,700)  | 1:5:A:ASP:HB2   | 1:6:A:LEU:H     | 7                   | 0.15     | 0.04                | 0.15       |
| (1,209)  | 1:61:A:LYS:HB3  | 1:61:A:LYS:HA   | 7                   | 0.12     | 0.01                | 0.11       |
| (1,1154) | 1:64:A:TYR:H    | 1:63:A:LEU:HD12 | 7                   | 0.11     | 0.01                | 0.12       |
| (1,916)  | 1:40:A:GLY:H    | 1:42:A:PHE:HD1  | 7                   | 0.11     | 0.01                | 0.11       |
| (1,384)  | 1:17:A:PRO:HA   | 1:18:A:GLN:HG2  | 6                   | 1.31     | 0.19                | 1.38       |
| (1,533)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HE1  | 6                   | 0.85     | 0.43                | 1.01       |
| (1,769)  | 1:22:A:GLU:H    | 1:21:A:ASP:HB3  | 6                   | 0.75     | 0.31                | 0.9        |
| (1,750)  | 1:19:A:ASN:H    | 1:18:A:GLN:HG2  | 6                   | 0.48     | 0.14                | 0.49       |
| (1,228)  | 1:65:A:LEU:HB2  | 1:65:A:LEU:HA   | 6                   | 0.41     | 0.02                | 0.42       |
| (1,965)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB3  | 6                   | 0.28     | 0.13                | 0.28       |
| (1,518)  | 1:33:A:VAL:HB   | 1:7:A:PHE:HB3   | 6                   | 0.14     | 0.04                | 0.12       |
| (1,1026) | 1:37:A:CYS:H    | 1:36:A:LYS:HB2  | 6                   | 0.14     | 0.03                | 0.14       |
| (1,1025) | 1:37:A:CYS:H    | 1:35:A:GLU:HG2  | 5                   | 1.28     | 0.2                 | 1.33       |
| (1,534)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HD1  | 5                   | 0.61     | 0.2                 | 0.74       |
| (1,845)  | 1:7:A:PHE:H     | 1:6:A:LEU:HD21  | 5                   | 0.53     | 0.27                | 0.73       |
| (1,845)  | 1:7:A:PHE:H     | 1:6:A:LEU:HD23  | 5                   | 0.53     | 0.27                | 0.73       |
| (1,845)  | 1:7:A:PHE:H     | 1:6:A:LEU:HD22  | 5                   | 0.53     | 0.27                | 0.73       |
| (1,289)  | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 5                   | 0.52     | 0.22                | 0.58       |
| (1,153)  | 1:49:A:THR:HG21 | 1:49:A:THR:HG1  | 5                   | 0.51     | 0.03                | 0.52       |
| (1,1159) | 1:65:A:LEU:H    | 1:65:A:LEU:HB2  | 5                   | 0.29     | 0.1                 | 0.27       |

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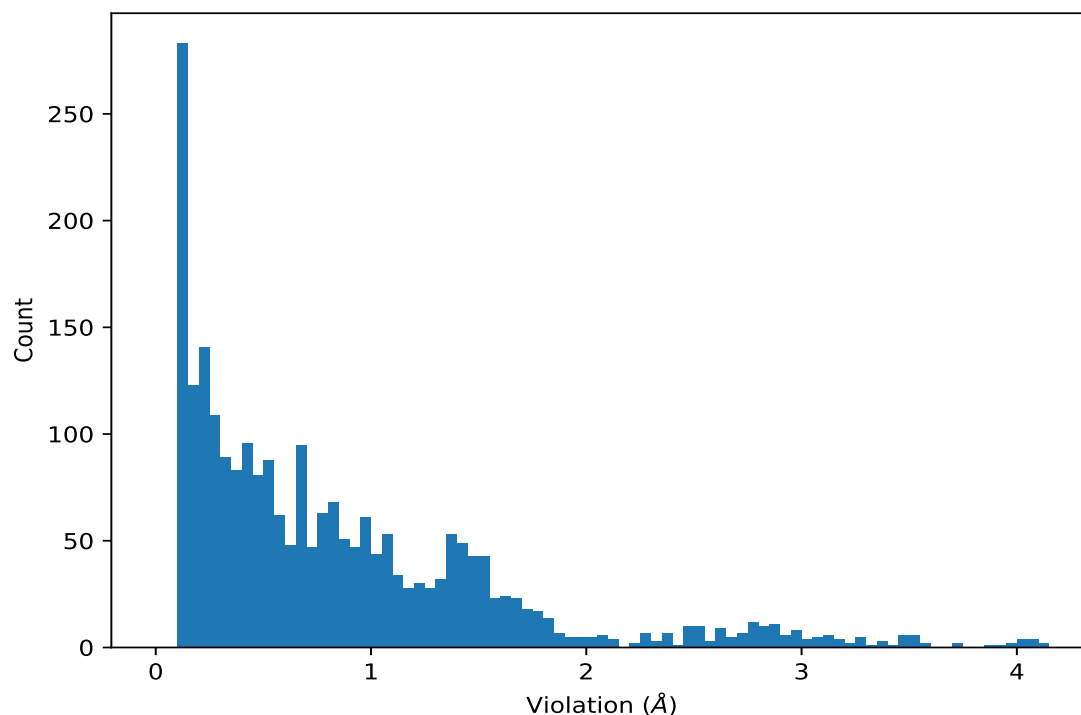
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,269)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG23 | 5                   | 0.26     | 0.06                | 0.26       |
| (1,269)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 5                   | 0.26     | 0.06                | 0.26       |
| (1,269)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG21 | 5                   | 0.26     | 0.06                | 0.26       |
| (1,501)  | 1:48:A:ARG:HA   | 1:48:A:ARG:HG2  | 5                   | 0.24     | 0.06                | 0.21       |
| (1,45)   | 1:21:A:ASP:HB2  | 1:21:A:ASP:HA   | 5                   | 0.23     | 0.01                | 0.23       |
| (1,762)  | 1:21:A:ASP:H    | 1:21:A:ASP:HB3  | 5                   | 0.16     | 0.02                | 0.16       |
| (1,943)  | 1:25:A:LEU:H    | 1:15:A:TYR:HB2  | 5                   | 0.13     | 0.03                | 0.12       |
| (1,837)  | 1:5:A:ASP:H     | 1:4:A:GLN:HB3   | 4                   | 1.06     | 0.55                | 1.36       |
| (1,299)  | 1:10:A:GLN:HG2  | 1:11:A:ALA:HB2  | 4                   | 0.56     | 0.15                | 0.51       |
| (1,1057) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 4                   | 0.53     | 0.04                | 0.55       |
| (1,831)  | 1:4:A:GLN:H     | 1:4:A:GLN:HG2   | 4                   | 0.42     | 0.13                | 0.46       |
| (1,587)  | 1:50:A:LYS:HE2  | 1:47:A:ARG:HA   | 4                   | 0.3      | 0.34                | 0.11       |
| (1,1062) | 1:48:A:ARG:H    | 1:47:A:ARG:HB2  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,899)  | 1:31:A:VAL:H    | 1:30:A:ILE:HG13 | 4                   | 0.13     | 0.01                | 0.12       |
| (1,87)   | 1:39:A:ASP:HB3  | 1:39:A:ASP:H    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,374)  | 1:16:A:ILE:HD12 | 1:14:A:SER:HB3  | 3                   | 0.85     | 0.14                | 0.81       |
| (1,250)  | 1:14:A:SER:HB3  | 1:15:A:TYR:H    | 3                   | 0.67     | 0.06                | 0.67       |
| (1,487)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE21 | 3                   | 0.48     | 0.19                | 0.47       |
| (1,65)   | 1:34:A:MET:HG2  | 1:35:A:GLU:HB2  | 3                   | 0.47     | 0.13                | 0.41       |
| (1,103)  | 1:42:A:PHE:HB3  | 1:33:A:VAL:HG22 | 3                   | 0.2      | 0.08                | 0.19       |
| (1,83)   | 1:38:A:ASP:HA   | 1:38:A:ASP:HB2  | 3                   | 0.18     | 0.0                 | 0.18       |
| (1,953)  | 1:26:A:ARG:H    | 1:15:A:TYR:H    | 3                   | 0.14     | 0.03                | 0.12       |
| (1,576)  | 1:49:A:THR:HB   | 1:46:A:SER:HB2  | 3                   | 0.13     | 0.04                | 0.1        |
| (1,510)  | 1:45:A:THR:HB   | 1:46:A:SER:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,244)  | 1:14:A:SER:HA   | 1:27:A:ASP:H    | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1045) | 1:46:A:SER:H    | 1:50:A:LYS:H    | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,332)  | 1:13:A:TYR:HB3  | 1:13:A:TYR:HD1  | 2                   | 1.19     | 0.0                 | 1.19       |
| (1,225)  | 1:65:A:LEU:HB3  | 1:5:A:ASP:HA    | 2                   | 0.77     | 0.2                 | 0.77       |
| (1,703)  | 1:7:A:PHE:H     | 1:7:A:PHE:HD2   | 2                   | 0.32     | 0.14                | 0.32       |
| (1,1015) | 1:36:A:LYS:H    | 1:35:A:GLU:HG2  | 2                   | 0.24     | 0.02                | 0.24       |
| (1,63)   | 1:34:A:MET:HB2  | 1:34:A:MET:HE2  | 2                   | 0.18     | 0.02                | 0.18       |
| (1,676)  | 1:11:A:ALA:H    | 1:10:A:GLN:HB3  | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1011) | 1:36:A:LYS:H    | 1:33:A:VAL:HG22 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,964)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,8)    | 1:23:A:LEU:HA   | 1:23:A:LEU:HD22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,560)  | 1:47:A:ARG:HD3  | 1:47:A:ARG:HA   | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,886)  | 1:45:A:THR:H    | 1:45:A:THR:HB   | 2                   | 0.11     | 0.0                 | 0.11       |

<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) |
|---------|--------------|----------------|----------|---------------|
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 6        | 4.14          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 15       | 4.11          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 8        | 4.09          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 11       | 4.09          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 1        | 4.06          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 13       | 4.06          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 4        | 4.04          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 5        | 4.04          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 12       | 4.04          |
| (1,882) | 1:45:A:THR:H | 1:52:A:PHE:HD2 | 3        | 4.03          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,882) | 1:45:A:THR:H    | 1:52:A:PHE:HD2 | 2        | 3.98          |
| (1,882) | 1:45:A:THR:H    | 1:52:A:PHE:HD2 | 14       | 3.95          |
| (1,882) | 1:45:A:THR:H    | 1:52:A:PHE:HD2 | 10       | 3.93          |
| (1,882) | 1:45:A:THR:H    | 1:52:A:PHE:HD2 | 7        | 3.88          |
| (1,882) | 1:45:A:THR:H    | 1:52:A:PHE:HD2 | 9        | 3.74          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 12       | 3.73          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 8        | 3.59          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 6        | 3.57          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 11       | 3.55          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 12       | 3.55          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 11       | 3.54          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 5        | 3.52          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 10       | 3.52          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 13       | 3.52          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 1        | 3.48          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 7        | 3.48          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 14       | 3.47          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 2        | 3.45          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 12       | 3.45          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 13       | 3.45          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 1        | 3.42          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 11       | 3.39          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 13       | 3.38          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 9        | 3.35          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 9        | 3.33          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 3        | 3.3           |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 15       | 3.28          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 10       | 3.27          |
| (1,625) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HD1  | 4        | 3.26          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 8        | 3.25          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 9        | 3.21          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 6        | 3.2           |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 10       | 3.19          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 9        | 3.19          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 4        | 3.18          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 5        | 3.17          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 8        | 3.15          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 3        | 3.13          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 14       | 3.13          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 9        | 3.13          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 14       | 3.1           |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 10       | 3.1           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 7        | 3.08          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 2        | 3.07          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 15       | 3.07          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 7        | 3.07          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 4        | 3.06          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 1        | 3.05          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 3        | 3.03          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 13       | 3.02          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 7        | 3.0           |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 10       | 2.99          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 11       | 2.99          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 15       | 2.98          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 9        | 2.97          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 6        | 2.97          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 8        | 2.97          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 11       | 2.96          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 13       | 2.95          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 5        | 2.94          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 4        | 2.94          |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1 | 2        | 2.93          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 1        | 2.92          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 3        | 2.92          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 2        | 2.91          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 9        | 2.9           |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 15       | 2.9           |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 6        | 2.89          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 12       | 2.89          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 12       | 2.88          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 5        | 2.87          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 10       | 2.85          |
| (1,624) | 1:57:A:GLY:HA3  | 1:9:A:TYR:HE1  | 4        | 2.85          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 11       | 2.85          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 2        | 2.85          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 12       | 2.85          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 7        | 2.84          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 5        | 2.84          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 13       | 2.84          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 4        | 2.83          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 2        | 2.83          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 1        | 2.82          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 2        | 2.81          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 13       | 2.81          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 4        | 2.81          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 15       | 2.81          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 6        | 2.8           |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 8        | 2.8           |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 14       | 2.79          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 8        | 2.79          |
| (1,483) | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2 | 1        | 2.78          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 7        | 2.77          |
| (1,645) | 1:60:A:VAL:HG22 | 1:9:A:TYR:HD1  | 8        | 2.76          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 6        | 2.76          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 7        | 2.76          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 11       | 2.75          |
| (1,483) | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2 | 13       | 2.75          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 3        | 2.75          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 1        | 2.73          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 3        | 2.72          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 11       | 2.71          |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 15       | 2.7           |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 3        | 2.7           |
| (1,272) | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3 | 11       | 2.7           |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 5        | 2.7           |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 11       | 2.69          |
| (1,483) | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2 | 15       | 2.69          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 2        | 2.69          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 2        | 2.68          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 5        | 2.67          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 10       | 2.65          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 12       | 2.65          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 14       | 2.65          |
| (1,483) | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2 | 4        | 2.63          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 3        | 2.62          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 1        | 2.61          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 13       | 2.61          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 15       | 2.61          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 7        | 2.6           |
| (1,546) | 1:45:A:THR:HG21 | 1:52:A:PHE:HD2 | 9        | 2.57          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 13       | 2.57          |
| (1,113) | 1:43:A:VAL:HG22 | 1:52:A:PHE:HD2 | 14       | 2.56          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 15       | 2.55          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 8        | 2.55          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 13       | 2.55          |
| (1,272) | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3 | 6        | 2.55          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 2        | 2.54          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 12       | 2.53          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 8        | 2.51          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 4        | 2.51          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 12       | 2.5           |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 5        | 2.5           |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 8        | 2.49          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 1        | 2.49          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 14       | 2.48          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 14       | 2.48          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 15       | 2.47          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 10       | 2.46          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 9        | 2.46          |
| (1,272) | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3 | 12       | 2.46          |
| (1,873) | 1:18:A:GLN:H    | 1:15:A:TYR:HE1 | 7        | 2.45          |
| (1,118) | 1:43:A:VAL:HG12 | 1:52:A:PHE:HD2 | 9        | 2.45          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 12       | 2.43          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 10       | 2.4           |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 11       | 2.4           |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 6        | 2.39          |
| (1,873) | 1:18:A:GLN:H    | 1:15:A:TYR:HE1 | 13       | 2.38          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 5        | 2.38          |
| (1,272) | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3 | 4        | 2.36          |
| (1,272) | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3 | 5        | 2.35          |
| (1,272) | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3 | 9        | 2.34          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 1        | 2.33          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 3        | 2.31          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 4        | 2.3           |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 10       | 2.3           |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 6        | 2.28          |
| (1,321) | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1 | 12       | 2.28          |
| (1,272) | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3 | 14       | 2.28          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 4        | 2.27          |
| (1,515) | 1:33:A:VAL:HB   | 1:9:A:TYR:HD1  | 7        | 2.26          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 6        | 2.22          |
| (1,516) | 1:33:A:VAL:HB   | 1:9:A:TYR:HE1  | 7        | 2.21          |
| (1,526) | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3 | 3        | 2.14          |
| (1,470) | 1:25:A:LEU:HD12 | 1:59:A:TYR:HE1 | 14       | 2.14          |
| (1,321) | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1 | 9        | 2.13          |
| (1,320) | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1 | 12       | 2.13          |
| (1,526) | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3 | 8        | 2.09          |
| (1,526) | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3 | 12       | 2.09          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,320)  | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 8        | 2.09          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 15       | 2.08          |
| (1,321)  | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1  | 11       | 2.07          |
| (1,321)  | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1  | 13       | 2.07          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 8        | 2.05          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 11       | 2.04          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 6        | 2.03          |
| (1,321)  | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1  | 8        | 2.03          |
| (1,321)  | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1  | 10       | 2.01          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 4        | 1.98          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 3        | 1.97          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 13       | 1.97          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 15       | 1.97          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 1        | 1.96          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 6        | 1.95          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 14       | 1.94          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 9        | 1.93          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 9        | 1.92          |
| (1,321)  | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1  | 7        | 1.92          |
| (1,321)  | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1  | 4        | 1.89          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 8        | 1.88          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 5        | 1.87          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 2        | 1.87          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 12       | 1.86          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 4        | 1.85          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 13       | 1.85          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 10       | 1.84          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 1        | 1.84          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 3        | 1.84          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 8        | 1.84          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 10       | 1.83          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 2        | 1.83          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 7        | 1.83          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 8        | 1.83          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 11       | 1.83          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 2        | 1.82          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 3        | 1.81          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 2        | 1.81          |
| (1,320)  | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 11       | 1.81          |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 7        | 1.8           |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 9        | 1.79          |
| (1,321)  | 1:12:A:LEU:HB2  | 1:13:A:TYR:HD1  | 2        | 1.79          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 10       | 1.79          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 15       | 1.78          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 3        | 1.78          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 13       | 1.78          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 15       | 1.78          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 1        | 1.77          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 2        | 1.77          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 2        | 1.77          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 6        | 1.77          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 7        | 1.76          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 14       | 1.76          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 12       | 1.76          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 4        | 1.75          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 13       | 1.75          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 5        | 1.75          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 11       | 1.74          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 11       | 1.74          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 10       | 1.74          |
| (1,320)  | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 9        | 1.74          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 6        | 1.73          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 1        | 1.73          |
| (1,320)  | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 10       | 1.73          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 12       | 1.73          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 10       | 1.73          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 7        | 1.72          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 11       | 1.72          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 14       | 1.72          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 7        | 1.71          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 2        | 1.71          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 6        | 1.71          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 15       | 1.71          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 9        | 1.71          |
| (1,320)  | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 13       | 1.71          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 5        | 1.7           |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 13       | 1.7           |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 4        | 1.7           |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 12       | 1.7           |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 15       | 1.7           |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 3        | 1.69          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 7        | 1.69          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 8        | 1.68          |
| (1,538)  | 1:37:A:CYS:HB2  | 1:40:A:GLY:H    | 4        | 1.68          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 15       | 1.68          |
| (1,1050) | 1:46:A:SER:H    | 1:23:A:LEU:HD22 | 12       | 1.67          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 15       | 1.67          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 3        | 1.67          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 5        | 1.67          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 9        | 1.67          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 6        | 1.67          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 1        | 1.66          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 3        | 1.66          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 6        | 1.66          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 8        | 1.66          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 10       | 1.66          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 5        | 1.66          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 10       | 1.66          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 8        | 1.65          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 12       | 1.65          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 10       | 1.64          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 2        | 1.64          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 4        | 1.64          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 11       | 1.64          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 12       | 1.63          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 13       | 1.63          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 1        | 1.63          |
| (1,1147) | 1:64:A:TYR:H    | 1:64:A:TYR:HD1  | 15       | 1.62          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 13       | 1.62          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 9        | 1.62          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 8        | 1.62          |
| (1,1147) | 1:64:A:TYR:H    | 1:64:A:TYR:HD1  | 10       | 1.61          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 7        | 1.61          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 14       | 1.61          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 13       | 1.61          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 10       | 1.61          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 14       | 1.61          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 4        | 1.61          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 1        | 1.6           |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 6        | 1.6           |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 12       | 1.6           |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 2        | 1.6           |
| (1,1035) | 1:44:A:GLY:H    | 1:52:A:PHE:HD2  | 14       | 1.59          |
| (1,586)  | 1:50:A:LYS:HE2  | 1:50:A:LYS:HA   | 13       | 1.59          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 1        | 1.59          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 7        | 1.59          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1025) | 1:37:A:CYS:H    | 1:35:A:GLU:HG2  | 9        | 1.58          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 5        | 1.58          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 2        | 1.58          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 12       | 1.58          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 2        | 1.58          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 8        | 1.57          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 5        | 1.57          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 8        | 1.57          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 10       | 1.57          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 12       | 1.57          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 9        | 1.57          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 11       | 1.56          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 15       | 1.56          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 5        | 1.56          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 1        | 1.56          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 9        | 1.56          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 1        | 1.56          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 2        | 1.55          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 3        | 1.55          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 13       | 1.54          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 13       | 1.54          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 11       | 1.54          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 13       | 1.54          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 7        | 1.54          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 11       | 1.54          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 14       | 1.54          |
| (1,590)  | 1:53:A:GLY:HA3  | 1:43:A:VAL:HG22 | 14       | 1.53          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 4        | 1.53          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 6        | 1.53          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 2        | 1.53          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 11       | 1.53          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 6        | 1.53          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 8        | 1.53          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 11       | 1.53          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 8        | 1.53          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 5        | 1.52          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 10       | 1.52          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 9        | 1.52          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 6        | 1.52          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 4        | 1.52          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 5        | 1.52          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 5        | 1.52          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 6        | 1.52          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 12       | 1.52          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 13       | 1.52          |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 5        | 1.52          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 3        | 1.52          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 4        | 1.52          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 9        | 1.51          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 2        | 1.51          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 13       | 1.51          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 14       | 1.51          |
| (1,320)  | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 4        | 1.51          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 11       | 1.51          |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 4        | 1.51          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 15       | 1.5           |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 4        | 1.5           |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 14       | 1.5           |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 15       | 1.5           |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 6        | 1.5           |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 3        | 1.5           |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 2        | 1.5           |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 5        | 1.49          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 1        | 1.49          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 11       | 1.49          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 14       | 1.49          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 1        | 1.49          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 11       | 1.49          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 14       | 1.49          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 2        | 1.49          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 9        | 1.49          |
| (1,384)  | 1:17:A:PRO:HA   | 1:18:A:GLN:HG2  | 9        | 1.49          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 12       | 1.49          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 13       | 1.49          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 11       | 1.48          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 2        | 1.48          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 3        | 1.48          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 6        | 1.48          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 5        | 1.48          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 15       | 1.48          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 3        | 1.48          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 15       | 1.48          |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 3        | 1.48          |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 12       | 1.48          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 14       | 1.48          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 3        | 1.47          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 12       | 1.47          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 15       | 1.47          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 11       | 1.47          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 7        | 1.47          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 8        | 1.47          |
| (1,384)  | 1:17:A:PRO:HA   | 1:18:A:GLN:HG2  | 4        | 1.47          |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 8        | 1.47          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 6        | 1.47          |
| (1,945)  | 1:26:A:ARG:H    | 1:25:A:LEU:HD22 | 11       | 1.46          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 9        | 1.46          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 7        | 1.46          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 9        | 1.46          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 13       | 1.46          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 3        | 1.46          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 4        | 1.46          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 8        | 1.46          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 10       | 1.46          |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 15       | 1.46          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 5        | 1.46          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 5        | 1.45          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 2        | 1.45          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 1        | 1.45          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 2        | 1.45          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 5        | 1.45          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 14       | 1.45          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 8        | 1.45          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 8        | 1.45          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 8        | 1.45          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 14       | 1.45          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 7        | 1.45          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 11       | 1.45          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 3        | 1.45          |
| (1,133)  | 1:51:A:GLN:HB3  | 1:23:A:LEU:HD22 | 13       | 1.45          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 12       | 1.44          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 5        | 1.44          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 6        | 1.44          |
| (1,483)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 9        | 1.44          |
| (1,466)  | 1:25:A:LEU:HD12 | 1:17:A:PRO:HG2  | 5        | 1.44          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 13       | 1.44          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 1        | 1.44          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,342) | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 6        | 1.44          |
| (1,205) | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 7        | 1.44          |
| (1,176) | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 10       | 1.44          |
| (1,998) | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 12       | 1.43          |
| (1,945) | 1:26:A:ARG:H    | 1:25:A:LEU:HD22 | 4        | 1.43          |
| (1,835) | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 3        | 1.43          |
| (1,520) | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 1        | 1.43          |
| (1,520) | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 3        | 1.43          |
| (1,451) | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 6        | 1.43          |
| (1,451) | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 11       | 1.43          |
| (1,384) | 1:17:A:PRO:HA   | 1:18:A:GLN:HG2  | 7        | 1.43          |
| (1,998) | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 10       | 1.42          |
| (1,578) | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 15       | 1.42          |
| (1,544) | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 14       | 1.42          |
| (1,506) | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 2        | 1.42          |
| (1,506) | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 3        | 1.42          |
| (1,451) | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 15       | 1.42          |
| (1,320) | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 7        | 1.42          |
| (1,176) | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 1        | 1.42          |
| (1,176) | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 11       | 1.42          |
| (1,144) | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 10       | 1.42          |
| (1,998) | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 13       | 1.41          |
| (1,520) | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 14       | 1.41          |
| (1,451) | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 2        | 1.41          |
| (1,451) | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 10       | 1.41          |
| (1,414) | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 1        | 1.41          |
| (1,176) | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 7        | 1.41          |
| (1,144) | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 13       | 1.41          |
| (1,998) | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 3        | 1.4           |
| (1,998) | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 14       | 1.4           |
| (1,873) | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 9        | 1.4           |
| (1,837) | 1:5:A:ASP:H     | 1:4:A:GLN:HB3   | 9        | 1.4           |
| (1,547) | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 7        | 1.4           |
| (1,520) | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 8        | 1.4           |
| (1,520) | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 15       | 1.4           |
| (1,483) | 1:30:A:ILE:HD12 | 1:10:A:GLN:HG2  | 10       | 1.4           |
| (1,451) | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 9        | 1.4           |
| (1,379) | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 10       | 1.4           |
| (1,176) | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 6        | 1.4           |
| (1,176) | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 9        | 1.4           |
| (1,998) | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 7        | 1.39          |
| (1,837) | 1:5:A:ASP:H     | 1:4:A:GLN:HB3   | 3        | 1.39          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 11       | 1.39          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 9        | 1.39          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 7        | 1.39          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 1        | 1.39          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 7        | 1.39          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 7        | 1.39          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 14       | 1.39          |
| (1,945)  | 1:26:A:ARG:H    | 1:25:A:LEU:HD22 | 15       | 1.38          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 14       | 1.38          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 6        | 1.38          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 4        | 1.38          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 9        | 1.38          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 12       | 1.38          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 15       | 1.38          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 9        | 1.38          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 11       | 1.38          |
| (1,1025) | 1:37:A:CYS:H    | 1:35:A:GLU:HG2  | 1        | 1.37          |
| (1,945)  | 1:26:A:ARG:H    | 1:25:A:LEU:HD22 | 8        | 1.37          |
| (1,547)  | 1:45:A:THR:HG21 | 1:51:A:GLN:H    | 10       | 1.37          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 10       | 1.37          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 6        | 1.37          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 7        | 1.37          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 13       | 1.37          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 15       | 1.37          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 15       | 1.36          |
| (1,945)  | 1:26:A:ARG:H    | 1:25:A:LEU:HD22 | 2        | 1.36          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 12       | 1.36          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 4        | 1.36          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 3        | 1.36          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 4        | 1.35          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 8        | 1.35          |
| (1,379)  | 1:17:A:PRO:HD2  | 1:16:A:ILE:HD12 | 9        | 1.35          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 13       | 1.35          |
| (1,320)  | 1:12:A:LEU:HB3  | 1:13:A:TYR:HD1  | 2        | 1.35          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 1        | 1.35          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 1        | 1.35          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 8        | 1.35          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 7        | 1.35          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 5        | 1.35          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 13       | 1.34          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 5        | 1.34          |
| (1,384)  | 1:17:A:PRO:HA   | 1:18:A:GLN:HG2  | 3        | 1.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,338)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 8        | 1.34          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 8        | 1.34          |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 14       | 1.34          |
| (1,1025) | 1:37:A:CYS:H    | 1:35:A:GLU:HG2  | 5        | 1.33          |
| (1,837)  | 1:5:A:ASP:H     | 1:4:A:GLN:HB3   | 10       | 1.33          |
| (1,506)  | 1:31:A:VAL:HG22 | 1:45:A:THR:H    | 12       | 1.33          |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 5        | 1.33          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 10       | 1.33          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 12       | 1.33          |
| (1,176)  | 1:53:A:GLY:HA3  | 1:54:A:THR:HG21 | 13       | 1.33          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 5        | 1.33          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 11       | 1.33          |
| (1,451)  | 1:23:A:LEU:HG   | 1:51:A:GLN:HB3  | 4        | 1.32          |
| (1,338)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 6        | 1.32          |
| (1,338)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 13       | 1.32          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 14       | 1.32          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 13       | 1.32          |
| (1,1147) | 1:64:A:TYR:H    | 1:64:A:TYR:HD1  | 13       | 1.31          |
| (1,1041) | 1:44:A:GLY:H    | 1:33:A:VAL:HG22 | 2        | 1.31          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 2        | 1.31          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 12       | 1.31          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 10       | 1.31          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 7        | 1.3           |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 8        | 1.3           |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 9        | 1.3           |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 13       | 1.3           |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 12       | 1.3           |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 1        | 1.3           |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 13       | 1.3           |
| (1,945)  | 1:26:A:ARG:H    | 1:25:A:LEU:HD22 | 12       | 1.29          |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 12       | 1.29          |
| (1,414)  | 1:46:A:SER:HA   | 1:23:A:LEU:HD22 | 5        | 1.29          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 1        | 1.29          |
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 10       | 1.28          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 7        | 1.28          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 11       | 1.28          |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 8        | 1.27          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 11       | 1.27          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 12       | 1.27          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 4        | 1.27          |
| (1,205)  | 1:60:A:VAL:HB   | 1:9:A:TYR:HD1   | 9        | 1.27          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 1        | 1.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,578)  | 1:46:A:SER:HB3  | 1:49:A:THR:HG21 | 3        | 1.26          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 2        | 1.26          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 5        | 1.26          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 5        | 1.26          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 8        | 1.26          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 6        | 1.26          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 11       | 1.25          |
| (1,533)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HE1  | 6        | 1.25          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 1        | 1.25          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 7        | 1.25          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 5        | 1.25          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 2        | 1.25          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 6        | 1.25          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 14       | 1.25          |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 8        | 1.25          |
| (1,998)  | 1:34:A:MET:H    | 1:33:A:VAL:HG22 | 9        | 1.24          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 3        | 1.24          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 13       | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 1        | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 3        | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 4        | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 7        | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 8        | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 9        | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 11       | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 12       | 1.24          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 15       | 1.24          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 4        | 1.24          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 4        | 1.24          |
| (1,533)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HE1  | 11       | 1.23          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 4        | 1.23          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 9        | 1.23          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 14       | 1.23          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 10       | 1.23          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 14       | 1.23          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 7        | 1.23          |
| (1,338)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 2        | 1.23          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 8        | 1.22          |
| (1,514)  | 1:33:A:VAL:HG22 | 1:33:A:VAL:HA   | 13       | 1.22          |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 2        | 1.22          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 11       | 1.22          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 9        | 1.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 6        | 1.21          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 12       | 1.21          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 6        | 1.21          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 4        | 1.2           |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 8        | 1.2           |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 10       | 1.2           |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 14       | 1.19          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 12       | 1.19          |
| (1,533)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HE1  | 4        | 1.19          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 10       | 1.19          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 7        | 1.19          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 2        | 1.19          |
| (1,332)  | 1:13:A:TYR:HB3  | 1:13:A:TYR:HD1  | 1        | 1.19          |
| (1,332)  | 1:13:A:TYR:HB3  | 1:13:A:TYR:HD1  | 5        | 1.19          |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 10       | 1.18          |
| (1,525)  | 1:34:A:MET:HB2  | 1:33:A:VAL:HA   | 15       | 1.18          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 8        | 1.18          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 15       | 1.18          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 8        | 1.18          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 3        | 1.18          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 8        | 1.18          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 15       | 1.18          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 15       | 1.18          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 13       | 1.17          |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 7        | 1.17          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 11       | 1.16          |
| (1,520)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HD1   | 6        | 1.16          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 11       | 1.16          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 15       | 1.16          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 5        | 1.16          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 2        | 1.16          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 12       | 1.15          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 6        | 1.15          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 13       | 1.15          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 8        | 1.15          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 10       | 1.15          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 6        | 1.14          |
| (1,945)  | 1:26:A:ARG:H    | 1:25:A:LEU:HD22 | 3        | 1.14          |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 14       | 1.14          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 3        | 1.14          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 5        | 1.14          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 5        | 1.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 9        | 1.13          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 2        | 1.13          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 9        | 1.13          |
| (1,1025) | 1:37:A:CYS:H    | 1:35:A:GLU:HG2  | 4        | 1.12          |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 11       | 1.12          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 6        | 1.12          |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 13       | 1.12          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 3        | 1.12          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 12       | 1.12          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 7        | 1.12          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 13       | 1.11          |
| (1,384)  | 1:17:A:PRO:HA   | 1:18:A:GLN:HG2  | 14       | 1.11          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 6        | 1.11          |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 2        | 1.11          |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 13       | 1.11          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 8        | 1.11          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 1        | 1.1           |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 11       | 1.1           |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 15       | 1.1           |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 6        | 1.1           |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 7        | 1.1           |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 7        | 1.1           |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 2        | 1.1           |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 13       | 1.09          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 13       | 1.09          |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 7        | 1.09          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 9        | 1.09          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 14       | 1.09          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 9        | 1.09          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 12       | 1.09          |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 1        | 1.09          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 9        | 1.09          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 1        | 1.09          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 2        | 1.09          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 10       | 1.09          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 7        | 1.08          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 11       | 1.08          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 4        | 1.08          |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 13       | 1.08          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 10       | 1.08          |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 4        | 1.08          |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 15       | 1.08          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 3        | 1.08          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 10       | 1.08          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 12       | 1.08          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 4        | 1.08          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 5        | 1.08          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 15       | 1.08          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 6        | 1.07          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 14       | 1.07          |
| (1,380)  | 1:16:A:ILE:HD12 | 1:17:A:PRO:HD3  | 9        | 1.07          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 10       | 1.07          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 8        | 1.07          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 14       | 1.07          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 1        | 1.06          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 8        | 1.06          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 10       | 1.06          |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 15       | 1.06          |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 4        | 1.06          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 3        | 1.06          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 4        | 1.06          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 2        | 1.06          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 4        | 1.06          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 14       | 1.06          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 7        | 1.06          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 13       | 1.06          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 1        | 1.06          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 4        | 1.05          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 6        | 1.05          |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 3        | 1.05          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 6        | 1.05          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 14       | 1.05          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 3        | 1.05          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 14       | 1.05          |
| (1,115)  | 1:43:A:VAL:HG22 | 1:44:A:GLY:H    | 11       | 1.05          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 9        | 1.05          |
| (1,1147) | 1:64:A:TYR:H    | 1:64:A:TYR:HD1  | 6        | 1.04          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 1        | 1.04          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 7        | 1.04          |
| (1,724)  | 1:13:A:TYR:H    | 1:13:A:TYR:HD1  | 2        | 1.04          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 9        | 1.04          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 1        | 1.04          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 3        | 1.04          |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 3        | 1.04          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,374)  | 1:16:A:ILE:HD12 | 1:14:A:SER:HB3  | 9        | 1.04          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 4        | 1.04          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 10       | 1.03          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 9        | 1.03          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 14       | 1.03          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 7        | 1.03          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 13       | 1.02          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 4        | 1.02          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 4        | 1.02          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 12       | 1.02          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 14       | 1.02          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 15       | 1.02          |
| (1,1025) | 1:37:A:CYS:H    | 1:35:A:GLU:HG2  | 12       | 1.02          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 2        | 1.02          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 4        | 1.02          |
| (1,1147) | 1:64:A:TYR:H    | 1:64:A:TYR:HD1  | 9        | 1.01          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 14       | 1.01          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 12       | 1.01          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 7        | 1.01          |
| (1,708)  | 1:8:A:SER:HB3   | 1:8:A:SER:H     | 4        | 1.01          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 8        | 1.01          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 5        | 1.01          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 7        | 1.01          |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 9        | 1.01          |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 3        | 1.01          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 4        | 1.01          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 12       | 1.0           |
| (1,708)  | 1:8:A:SER:HB3   | 1:8:A:SER:H     | 12       | 1.0           |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 1        | 1.0           |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 2        | 1.0           |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 9        | 1.0           |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 10       | 1.0           |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 1        | 1.0           |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 8        | 1.0           |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 6        | 1.0           |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 10       | 1.0           |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 10       | 0.99          |
| (1,769)  | 1:22:A:GLU:H    | 1:21:A:ASP:HB3  | 13       | 0.99          |
| (1,708)  | 1:8:A:SER:HB3   | 1:8:A:SER:H     | 11       | 0.99          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 10       | 0.99          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 6        | 0.99          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 11       | 0.99          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 2        | 0.99          |
| (1,384)  | 1:17:A:PRO:HA   | 1:18:A:GLN:HG2  | 12       | 0.99          |
| (1,312)  | 1:12:A:LEU:HA   | 1:12:A:LEU:HD22 | 7        | 0.99          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 13       | 0.99          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 14       | 0.99          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 5        | 0.98          |
| (1,769)  | 1:22:A:GLU:H    | 1:21:A:ASP:HB3  | 4        | 0.98          |
| (1,708)  | 1:8:A:SER:HB3   | 1:8:A:SER:H     | 5        | 0.98          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 6        | 0.98          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 3        | 0.98          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 4        | 0.98          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 9        | 0.98          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 12       | 0.98          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 13       | 0.98          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 1        | 0.98          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 7        | 0.98          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 2        | 0.98          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 10       | 0.98          |
| (1,300)  | 1:10:A:GLN:HG2  | 1:61:A:LYS:HG3  | 10       | 0.98          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 15       | 0.98          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 10       | 0.97          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 14       | 0.97          |
| (1,708)  | 1:8:A:SER:HB3   | 1:8:A:SER:H     | 9        | 0.97          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 1        | 0.97          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 6        | 0.97          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 8        | 0.97          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 13       | 0.97          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 15       | 0.97          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 5        | 0.97          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 15       | 0.97          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 12       | 0.97          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 5        | 0.97          |
| (1,338)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 14       | 0.97          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 11       | 0.97          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 14       | 0.97          |
| (1,225)  | 1:65:A:LEU:HB3  | 1:5:A:ASP:HA    | 10       | 0.97          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 3        | 0.97          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 9        | 0.97          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 6        | 0.97          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 1        | 0.97          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 13       | 0.96          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 2        | 0.96          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 6        | 0.96          |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 2        | 0.96          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 4        | 0.96          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 12       | 0.96          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 15       | 0.96          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 11       | 0.96          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 12       | 0.96          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 5        | 0.96          |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 13       | 0.96          |
| (1,300)  | 1:10:A:GLN:HG2  | 1:61:A:LYS:HG3  | 9        | 0.96          |
| (1,300)  | 1:10:A:GLN:HG2  | 1:61:A:LYS:HG3  | 12       | 0.96          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 8        | 0.96          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 13       | 0.96          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 8        | 0.95          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 11       | 0.95          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 5        | 0.95          |
| (1,708)  | 1:8:A:SER:HB3   | 1:8:A:SER:H     | 6        | 0.95          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 10       | 0.95          |
| (1,646)  | 1:60:A:VAL:HG22 | 1:61:A:LYS:H    | 14       | 0.95          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 11       | 0.95          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 7        | 0.95          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 1        | 0.95          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 10       | 0.95          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 12       | 0.95          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 2        | 0.94          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 10       | 0.94          |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 7        | 0.94          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 13       | 0.94          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 14       | 0.94          |
| (1,129)  | 1:45:A:THR:HB   | 1:32:A:ASP:HB2  | 2        | 0.94          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 9        | 0.94          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 11       | 0.94          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 14       | 0.93          |
| (1,769)  | 1:22:A:GLU:H    | 1:21:A:ASP:HB3  | 15       | 0.93          |
| (1,708)  | 1:8:A:SER:HB3   | 1:8:A:SER:H     | 14       | 0.93          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 5        | 0.93          |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 6        | 0.93          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 8        | 0.93          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 9        | 0.92          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 15       | 0.92          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 3        | 0.92          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 9        | 0.92          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 13       | 0.92          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 14       | 0.92          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 4        | 0.92          |
| (1,410)  | 1:19:A:ASN:HB3  | 1:22:A:GLU:H    | 1        | 0.92          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 14       | 0.92          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 10       | 0.92          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 13       | 0.92          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 14       | 0.91          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 1        | 0.91          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 11       | 0.91          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 8        | 0.91          |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 2        | 0.91          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 3        | 0.91          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 3        | 0.9           |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 12       | 0.9           |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 13       | 0.9           |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 7        | 0.9           |
| (1,129)  | 1:45:A:THR:HB   | 1:32:A:ASP:HB2  | 14       | 0.9           |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 2        | 0.89          |
| (1,587)  | 1:50:A:LYS:HE2  | 1:47:A:ARG:HA   | 13       | 0.89          |
| (1,405)  | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 1        | 0.89          |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 6        | 0.89          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 5        | 0.89          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 15       | 0.89          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 1        | 0.89          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 9        | 0.88          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 13       | 0.88          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 15       | 0.88          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 3        | 0.88          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 9        | 0.88          |
| (1,937)  | 1:41:A:TRP:H    | 1:37:A:CYS:HB2  | 4        | 0.88          |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 1        | 0.88          |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 2        | 0.88          |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 13       | 0.88          |
| (1,769)  | 1:22:A:GLU:H    | 1:21:A:ASP:HB3  | 10       | 0.88          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 15       | 0.88          |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 8        | 0.88          |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 15       | 0.88          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 15       | 0.88          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 3        | 0.88          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 12       | 0.88          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 13       | 0.88          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,20)   | 1:24:A:GLU:HG2 | 1:16:A:ILE:HD12 | 1        | 0.88          |
| (1,1120) | 1:59:A:TYR:H   | 1:59:A:TYR:HD1  | 12       | 0.87          |
| (1,1058) | 1:48:A:ARG:H   | 1:49:A:THR:HG21 | 7        | 0.87          |
| (1,1000) | 1:35:A:GLU:H   | 1:33:A:VAL:HG22 | 6        | 0.87          |
| (1,913)  | 1:42:A:PHE:H   | 1:42:A:PHE:HB3  | 9        | 0.87          |
| (1,913)  | 1:42:A:PHE:H   | 1:42:A:PHE:HB3  | 14       | 0.87          |
| (1,555)  | 1:46:A:SER:HB2 | 1:49:A:THR:HG21 | 14       | 0.87          |
| (1,292)  | 1:10:A:GLN:HA  | 1:30:A:ILE:HD12 | 4        | 0.87          |
| (1,292)  | 1:10:A:GLN:HA  | 1:30:A:ILE:HD12 | 9        | 0.87          |
| (1,292)  | 1:10:A:GLN:HA  | 1:30:A:ILE:HD12 | 10       | 0.87          |
| (1,248)  | 1:46:A:SER:HB3 | 1:23:A:LEU:HD22 | 2        | 0.87          |
| (1,119)  | 1:44:A:GLY:HA3 | 1:33:A:VAL:HG22 | 5        | 0.87          |
| (1,11)   | 1:35:A:GLU:HA  | 1:35:A:GLU:HG2  | 4        | 0.87          |
| (1,1121) | 1:59:A:TYR:H   | 1:59:A:TYR:HE1  | 3        | 0.86          |
| (1,1121) | 1:59:A:TYR:H   | 1:59:A:TYR:HE1  | 12       | 0.86          |
| (1,1120) | 1:59:A:TYR:H   | 1:59:A:TYR:HD1  | 2        | 0.86          |
| (1,1096) | 1:51:A:GLN:H   | 1:23:A:LEU:HD22 | 15       | 0.86          |
| (1,1058) | 1:48:A:ARG:H   | 1:49:A:THR:HG21 | 10       | 0.86          |
| (1,913)  | 1:42:A:PHE:H   | 1:42:A:PHE:HB3  | 3        | 0.86          |
| (1,913)  | 1:42:A:PHE:H   | 1:42:A:PHE:HB3  | 8        | 0.86          |
| (1,913)  | 1:42:A:PHE:H   | 1:42:A:PHE:HB3  | 12       | 0.86          |
| (1,555)  | 1:46:A:SER:HB2 | 1:49:A:THR:HG21 | 2        | 0.86          |
| (1,555)  | 1:46:A:SER:HB2 | 1:49:A:THR:HG21 | 5        | 0.86          |
| (1,303)  | 1:11:A:ALA:HB2 | 1:28:A:GLY:HA3  | 10       | 0.86          |
| (1,303)  | 1:11:A:ALA:HB2 | 1:28:A:GLY:HA3  | 15       | 0.86          |
| (1,144)  | 1:48:A:ARG:HD3 | 1:48:A:ARG:HB2  | 5        | 0.86          |
| (1,11)   | 1:35:A:GLU:HA  | 1:35:A:GLU:HG2  | 12       | 0.86          |
| (1,1096) | 1:51:A:GLN:H   | 1:23:A:LEU:HD22 | 3        | 0.85          |
| (1,1058) | 1:48:A:ARG:H   | 1:49:A:THR:HG21 | 1        | 0.85          |
| (1,923)  | 1:52:A:PHE:H   | 1:45:A:THR:HG21 | 3        | 0.85          |
| (1,555)  | 1:46:A:SER:HB2 | 1:49:A:THR:HG21 | 1        | 0.85          |
| (1,303)  | 1:11:A:ALA:HB2 | 1:28:A:GLY:HA3  | 7        | 0.85          |
| (1,292)  | 1:10:A:GLN:HA  | 1:30:A:ILE:HD12 | 11       | 0.85          |
| (1,248)  | 1:46:A:SER:HB3 | 1:23:A:LEU:HD22 | 1        | 0.85          |
| (1,144)  | 1:48:A:ARG:HD3 | 1:48:A:ARG:HB2  | 8        | 0.85          |
| (1,119)  | 1:44:A:GLY:HA3 | 1:33:A:VAL:HG22 | 7        | 0.85          |
| (1,1114) | 1:55:A:PHE:H   | 1:54:A:THR:HG21 | 5        | 0.84          |
| (1,1114) | 1:55:A:PHE:H   | 1:54:A:THR:HG21 | 12       | 0.84          |
| (1,1058) | 1:48:A:ARG:H   | 1:49:A:THR:HG21 | 9        | 0.84          |
| (1,1032) | 1:43:A:VAL:H   | 1:33:A:VAL:HG22 | 5        | 0.84          |
| (1,923)  | 1:52:A:PHE:H   | 1:45:A:THR:HG21 | 9        | 0.84          |
| (1,913)  | 1:42:A:PHE:H   | 1:42:A:PHE:HB3  | 11       | 0.84          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 15       | 0.84          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 13       | 0.84          |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 9        | 0.84          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 14       | 0.84          |
| (1,533)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HE1  | 1        | 0.84          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 10       | 0.84          |
| (1,489)  | 1:30:A:ILE:HD12 | 1:11:A:ALA:H    | 5        | 0.84          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 13       | 0.84          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 7        | 0.84          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 12       | 0.84          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 3        | 0.84          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 9        | 0.83          |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 6        | 0.83          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 2        | 0.83          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 5        | 0.83          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 11       | 0.83          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 4        | 0.83          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 14       | 0.83          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 5        | 0.83          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 11       | 0.82          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 2        | 0.82          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 5        | 0.82          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 7        | 0.82          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 14       | 0.82          |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 7        | 0.82          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 3        | 0.82          |
| (1,299)  | 1:10:A:GLN:HG2  | 1:11:A:ALA:HB2  | 13       | 0.82          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 13       | 0.82          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 2        | 0.82          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 9        | 0.82          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 3        | 0.81          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 15       | 0.81          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 11       | 0.81          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 14       | 0.81          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 3        | 0.81          |
| (1,374)  | 1:16:A:ILE:HD12 | 1:14:A:SER:HB3  | 1        | 0.81          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 15       | 0.81          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 6        | 0.81          |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 14       | 0.81          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 9        | 0.81          |
| (1,129)  | 1:45:A:THR:HB   | 1:32:A:ASP:HB2  | 10       | 0.81          |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 6        | 0.8           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 3        | 0.8           |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 13       | 0.8           |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 8        | 0.8           |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 3        | 0.8           |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 10       | 0.8           |
| (1,555)  | 1:46:A:SER:HB2  | 1:49:A:THR:HG21 | 11       | 0.8           |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 1        | 0.8           |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 4        | 0.8           |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 3        | 0.8           |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 12       | 0.8           |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 15       | 0.8           |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 15       | 0.79          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 3        | 0.79          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 9        | 0.79          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 3        | 0.79          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 7        | 0.79          |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 7        | 0.79          |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 10       | 0.79          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 7        | 0.79          |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 5        | 0.79          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 7        | 0.79          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 8        | 0.79          |
| (1,373)  | 1:16:A:ILE:HD12 | 1:24:A:GLU:HG3  | 11       | 0.79          |
| (1,300)  | 1:10:A:GLN:HG2  | 1:61:A:LYS:HG3  | 3        | 0.79          |
| (1,129)  | 1:45:A:THR:HB   | 1:32:A:ASP:HB2  | 13       | 0.79          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 8        | 0.78          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 8        | 0.78          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 8        | 0.78          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 10       | 0.78          |
| (1,694)  | 1:16:A:ILE:H    | 1:16:A:ILE:HD12 | 7        | 0.78          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 14       | 0.78          |
| (1,534)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HD1  | 4        | 0.78          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 3        | 0.78          |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 12       | 0.78          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 3        | 0.78          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 13       | 0.77          |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 5        | 0.77          |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 11       | 0.77          |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 13       | 0.77          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 2        | 0.77          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 11       | 0.76          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 12       | 0.76          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 1        | 0.76          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 14       | 0.76          |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 4        | 0.76          |
| (1,913)  | 1:42:A:PHE:H    | 1:42:A:PHE:HB3  | 5        | 0.76          |
| (1,845)  | 1:7:A:PHE:H     | 1:6:A:LEU:HD22  | 12       | 0.76          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 11       | 0.76          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 1        | 0.76          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 6        | 0.76          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 14       | 0.76          |
| (1,292)  | 1:10:A:GLN:HA   | 1:30:A:ILE:HD12 | 5        | 0.76          |
| (1,248)  | 1:46:A:SER:HB3  | 1:23:A:LEU:HD22 | 5        | 0.76          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 2        | 0.76          |
| (1,166)  | 1:51:A:GLN:HB2  | 1:49:A:THR:HG1  | 4        | 0.76          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 2        | 0.76          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 6        | 0.75          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 10       | 0.75          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 10       | 0.75          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 6        | 0.75          |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 6        | 0.75          |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 8        | 0.75          |
| (1,534)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HD1  | 6        | 0.75          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 5        | 0.75          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 1        | 0.75          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 7        | 0.75          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 9        | 0.75          |
| (1,289)  | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 13       | 0.75          |
| (1,250)  | 1:14:A:SER:HB3  | 1:15:A:TYR:H    | 1        | 0.75          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 12       | 0.75          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 13       | 0.75          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 14       | 0.75          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 6        | 0.75          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 13       | 0.75          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 5        | 0.74          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 7        | 0.74          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 7        | 0.74          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 4        | 0.74          |
| (1,845)  | 1:7:A:PHE:H     | 1:6:A:LEU:HD23  | 7        | 0.74          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 1        | 0.74          |
| (1,534)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HD1  | 11       | 0.74          |
| (1,129)  | 1:45:A:THR:HB   | 1:32:A:ASP:HB2  | 9        | 0.74          |
| (1,119)  | 1:44:A:GLY:HA3  | 1:33:A:VAL:HG22 | 12       | 0.74          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 14       | 0.74          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 12       | 0.73          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 8        | 0.73          |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 10       | 0.73          |
| (1,845)  | 1:7:A:PHE:H     | 1:6:A:LEU:HD21  | 8        | 0.73          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 12       | 0.73          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 8        | 0.73          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 13       | 0.73          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 5        | 0.73          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 13       | 0.73          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 4        | 0.73          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 1        | 0.72          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 4        | 0.72          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 9        | 0.72          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 7        | 0.72          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 7        | 0.72          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 13       | 0.72          |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 10       | 0.72          |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 12       | 0.72          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 10       | 0.72          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 11       | 0.72          |
| (1,487)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE21 | 5        | 0.72          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 8        | 0.72          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 5        | 0.72          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 5        | 0.72          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 8        | 0.71          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 10       | 0.71          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 4        | 0.71          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 7        | 0.71          |
| (1,923)  | 1:52:A:PHE:H    | 1:45:A:THR:HG21 | 15       | 0.71          |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 15       | 0.71          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 12       | 0.71          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 6        | 0.71          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 15       | 0.71          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 7        | 0.71          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 15       | 0.71          |
| (1,303)  | 1:11:A:ALA:HB2  | 1:28:A:GLY:HA3  | 8        | 0.71          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 8        | 0.71          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 3        | 0.7           |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 6        | 0.7           |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 15       | 0.7           |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 7        | 0.7           |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 6        | 0.7           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 3        | 0.7           |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 9        | 0.7           |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 12       | 0.7           |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 13       | 0.7           |
| (1,662)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HD1  | 9        | 0.7           |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 6        | 0.7           |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 4        | 0.7           |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 15       | 0.7           |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 15       | 0.7           |
| (1,374)  | 1:16:A:ILE:HD12 | 1:14:A:SER:HB3  | 8        | 0.7           |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 10       | 0.7           |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 11       | 0.69          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 6        | 0.69          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 14       | 0.69          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 2        | 0.69          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 6        | 0.69          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 11       | 0.69          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 8        | 0.69          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 9        | 0.69          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 9        | 0.69          |
| (1,300)  | 1:10:A:GLN:HG2  | 1:61:A:LYS:HG3  | 8        | 0.69          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 1        | 0.69          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 15       | 0.69          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 4        | 0.69          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 7        | 0.69          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 13       | 0.68          |
| (1,1121) | 1:59:A:TYR:H    | 1:59:A:TYR:HE1  | 5        | 0.68          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 6        | 0.68          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 8        | 0.68          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 2        | 0.68          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 11       | 0.68          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 14       | 0.68          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 12       | 0.68          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 4        | 0.68          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 5        | 0.68          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 7        | 0.68          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 6        | 0.68          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 15       | 0.67          |
| (1,1058) | 1:48:A:ARG:H    | 1:49:A:THR:HG21 | 4        | 0.67          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 15       | 0.67          |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 11       | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 1        | 0.67          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 3        | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 4        | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 5        | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 7        | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 8        | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 9        | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 10       | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 12       | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 13       | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 14       | 0.67          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 15       | 0.67          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 1        | 0.67          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 6        | 0.67          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 10       | 0.67          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 11       | 0.67          |
| (1,300)  | 1:10:A:GLN:HG2  | 1:61:A:LYS:HG3  | 6        | 0.67          |
| (1,250)  | 1:14:A:SER:HB3  | 1:15:A:TYR:H    | 9        | 0.67          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 6        | 0.67          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 15       | 0.67          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 6        | 0.67          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 11       | 0.67          |
| (1,1120) | 1:59:A:TYR:H    | 1:59:A:TYR:HD1  | 5        | 0.66          |
| (1,1114) | 1:55:A:PHE:H    | 1:54:A:THR:HG21 | 8        | 0.66          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 1        | 0.66          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 1        | 0.66          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 8        | 0.66          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 14       | 0.66          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 2        | 0.66          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 11       | 0.66          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 14       | 0.66          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 4        | 0.66          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 5        | 0.66          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 13       | 0.66          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 9        | 0.66          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 8        | 0.66          |
| (1,70)   | 1:35:A:GLU:HB2  | 1:34:A:MET:HE2  | 10       | 0.66          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 3        | 0.66          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 2        | 0.65          |
| (1,1133) | 1:60:A:VAL:H    | 1:60:A:VAL:HG22 | 14       | 0.65          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 2        | 0.65          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 10       | 0.65          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 1        | 0.65          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 6        | 0.65          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 11       | 0.65          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 1        | 0.65          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 12       | 0.65          |
| (1,65)   | 1:34:A:MET:HG2  | 1:35:A:GLU:HB2  | 13       | 0.65          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 13       | 0.65          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 15       | 0.64          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 8        | 0.64          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 13       | 0.64          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 8        | 0.64          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 3        | 0.64          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 7        | 0.64          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 9        | 0.64          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 10       | 0.64          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 12       | 0.64          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 8        | 0.64          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 12       | 0.64          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 3        | 0.64          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 10       | 0.64          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 12       | 0.64          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 11       | 0.64          |
| (1,788)  | 1:25:A:LEU:H    | 1:15:A:TYR:HD1  | 12       | 0.63          |
| (1,750)  | 1:19:A:ASN:H    | 1:18:A:GLN:HG2  | 9        | 0.63          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 1        | 0.63          |
| (1,526)  | 1:34:A:MET:HG2  | 1:44:A:GLY:HA3  | 13       | 0.63          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 2        | 0.63          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 8        | 0.63          |
| (1,1147) | 1:64:A:TYR:H    | 1:64:A:TYR:HD1  | 7        | 0.62          |
| (1,1032) | 1:43:A:VAL:H    | 1:33:A:VAL:HG22 | 2        | 0.62          |
| (1,750)  | 1:19:A:ASN:H    | 1:18:A:GLN:HG2  | 7        | 0.62          |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 6        | 0.62          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 2        | 0.62          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 12       | 0.62          |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 10       | 0.62          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 9        | 0.62          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 10       | 0.62          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 14       | 0.62          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 11       | 0.62          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 8        | 0.62          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 9        | 0.62          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 2        | 0.62          |
| (1,129)  | 1:45:A:THR:HB   | 1:32:A:ASP:HB2  | 5        | 0.62          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 3        | 0.62          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 3        | 0.61          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 9        | 0.61          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 1        | 0.61          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 8        | 0.61          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 3        | 0.61          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 15       | 0.61          |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 1        | 0.61          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 2        | 0.61          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 6        | 0.61          |
| (1,289)  | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 4        | 0.61          |
| (1,12)   | 1:35:A:GLU:HA   | 1:36:A:LYS:HG2  | 9        | 0.61          |
| (1,769)  | 1:22:A:GLU:H    | 1:21:A:ASP:HB3  | 8        | 0.6           |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 4        | 0.6           |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 10       | 0.6           |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 15       | 0.6           |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 1        | 0.6           |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 11       | 0.6           |
| (1,250)  | 1:14:A:SER:HB3  | 1:15:A:TYR:H    | 8        | 0.6           |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 1        | 0.6           |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 2        | 0.6           |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 1        | 0.6           |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 1        | 0.59          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 9        | 0.59          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 4        | 0.59          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 8        | 0.59          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 4        | 0.59          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 5        | 0.59          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 11       | 0.59          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 15       | 0.59          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 4        | 0.58          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 7        | 0.58          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 12       | 0.58          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 1        | 0.58          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 2        | 0.58          |
| (1,289)  | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 1        | 0.58          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 13       | 0.57          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 15       | 0.57          |
| (1,810)  | 1:43:A:VAL:H    | 1:42:A:PHE:HB2  | 5        | 0.57          |
| (1,760)  | 1:20:A:ASP:H    | 1:19:A:ASN:HB3  | 1        | 0.57          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 10       | 0.57          |
| (1,638)  | 1:60:A:VAL:HA   | 1:9:A:TYR:HD1   | 9        | 0.57          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 3        | 0.57          |
| (1,469)  | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 4        | 0.57          |
| (1,225)  | 1:65:A:LEU:HB3  | 1:5:A:ASP:HA    | 7        | 0.57          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 11       | 0.57          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 12       | 0.57          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 6        | 0.57          |
| (1,1057) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 7        | 0.56          |
| (1,831)  | 1:4:A:GLN:H     | 1:4:A:GLN:HG2   | 5        | 0.56          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 15       | 0.56          |
| (1,750)  | 1:19:A:ASN:H    | 1:18:A:GLN:HG2  | 3        | 0.56          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 4        | 0.56          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 5        | 0.56          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 6        | 0.56          |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 3        | 0.56          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 2        | 0.56          |
| (1,289)  | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 15       | 0.56          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 3        | 0.56          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 9        | 0.56          |
| (1,1147) | 1:64:A:TYR:H    | 1:64:A:TYR:HD1  | 12       | 0.55          |
| (1,1057) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 11       | 0.55          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 5        | 0.55          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 8        | 0.55          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 8        | 0.55          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 9        | 0.55          |
| (1,595)  | 1:22:A:GLU:HG3  | 1:54:A:THR:HG21 | 9        | 0.55          |
| (1,544)  | 1:44:A:GLY:HA3  | 1:32:A:ASP:HB2  | 11       | 0.55          |
| (1,534)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HD1  | 1        | 0.55          |
| (1,488)  | 1:30:A:ILE:HD12 | 1:31:A:VAL:H    | 5        | 0.55          |
| (1,299)  | 1:10:A:GLN:HG2  | 1:11:A:ALA:HB2  | 4        | 0.55          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 7        | 0.55          |
| (1,172)  | 1:52:A:PHE:HB3  | 1:45:A:THR:HG21 | 15       | 0.55          |
| (1,153)  | 1:49:A:THR:HG21 | 1:49:A:THR:HG1  | 11       | 0.55          |
| (1,1057) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 13       | 0.54          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 3        | 0.54          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 1        | 0.54          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 3        | 0.54          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 7        | 0.54          |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 7        | 0.54          |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 10       | 0.54          |
| (1,425)  | 1:33:A:VAL:HG22 | 1:42:A:PHE:HB2  | 4        | 0.54          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 10       | 0.54          |
| (1,110)  | 1:43:A:VAL:HG22 | 1:34:A:MET:HG2  | 2        | 0.54          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,997) | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 15       | 0.53          |
| (1,777) | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 6        | 0.53          |
| (1,647) | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 2        | 0.53          |
| (1,647) | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 15       | 0.53          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 6        | 0.53          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 8        | 0.53          |
| (1,153) | 1:49:A:THR:HG21 | 1:49:A:THR:HG1  | 15       | 0.53          |
| (1,84)  | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 1        | 0.53          |
| (1,84)  | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 5        | 0.53          |
| (1,84)  | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 8        | 0.53          |
| (1,84)  | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 12       | 0.53          |
| (1,37)  | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 7        | 0.53          |
| (1,20)  | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 2        | 0.53          |
| (1,997) | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 11       | 0.52          |
| (1,997) | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 12       | 0.52          |
| (1,647) | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 6        | 0.52          |
| (1,469) | 1:25:A:LEU:HD12 | 1:15:A:TYR:HD1  | 11       | 0.52          |
| (1,454) | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 10       | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 1        | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 2        | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 3        | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 4        | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 5        | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 7        | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 9        | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 10       | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 11       | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 12       | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 13       | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 14       | 0.52          |
| (1,372) | 1:16:A:ILE:HD12 | 1:16:A:ILE:HB   | 15       | 0.52          |
| (1,206) | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 1        | 0.52          |
| (1,206) | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 5        | 0.52          |
| (1,206) | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 6        | 0.52          |
| (1,206) | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 7        | 0.52          |
| (1,206) | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 11       | 0.52          |
| (1,206) | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 12       | 0.52          |
| (1,153) | 1:49:A:THR:HG21 | 1:49:A:THR:HG1  | 1        | 0.52          |
| (1,84)  | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 3        | 0.52          |
| (1,84)  | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 4        | 0.52          |
| (1,84)  | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 7        | 0.52          |
| (1,84)  | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 11       | 0.52          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,84)   | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 13       | 0.52          |
| (1,84)   | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 14       | 0.52          |
| (1,84)   | 1:39:A:ASP:HA   | 1:39:A:ASP:HB3  | 15       | 0.52          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 10       | 0.52          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 12       | 0.52          |
| (1,1096) | 1:51:A:GLN:H    | 1:23:A:LEU:HD22 | 5        | 0.51          |
| (1,1000) | 1:35:A:GLU:H    | 1:33:A:VAL:HG22 | 2        | 0.51          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 1        | 0.51          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 6        | 0.51          |
| (1,965)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB3  | 3        | 0.51          |
| (1,565)  | 1:50:A:LYS:HD2  | 1:50:A:LYS:HE2  | 13       | 0.51          |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 6        | 0.51          |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 11       | 0.51          |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 14       | 0.51          |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 3        | 0.51          |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 4        | 0.51          |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 8        | 0.51          |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 9        | 0.51          |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 10       | 0.51          |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 13       | 0.51          |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 14       | 0.51          |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 15       | 0.51          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 1        | 0.51          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 3        | 0.5           |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 4        | 0.5           |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 9        | 0.5           |
| (1,831)  | 1:4:A:GLN:H     | 1:4:A:GLN:HG2   | 7        | 0.5           |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 1        | 0.5           |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 8        | 0.5           |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 12       | 0.5           |
| (1,533)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HE1  | 13       | 0.5           |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 1        | 0.5           |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 2        | 0.5           |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 12       | 0.5           |
| (1,206)  | 1:60:A:VAL:HA   | 1:60:A:VAL:HG22 | 2        | 0.5           |
| (1,153)  | 1:49:A:THR:HG21 | 1:49:A:THR:HG1  | 5        | 0.5           |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 7        | 0.49          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 10       | 0.49          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 11       | 0.49          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 14       | 0.49          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 13       | 0.49          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 14       | 0.49          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 3        | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 5        | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 6        | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 7        | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 8        | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 9        | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 10       | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 11       | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 13       | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 14       | 0.49          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 15       | 0.49          |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 3        | 0.49          |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 2        | 0.49          |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 11       | 0.49          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 14       | 0.49          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 4        | 0.49          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 8        | 0.49          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 13       | 0.48          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 14       | 0.48          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 9        | 0.48          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 7        | 0.48          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 1        | 0.48          |
| (1,492)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HG13 | 4        | 0.48          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 6        | 0.48          |
| (1,272)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HB3  | 10       | 0.48          |
| (1,1159) | 1:65:A:LEU:H    | 1:65:A:LEU:HB2  | 10       | 0.47          |
| (1,1057) | 1:48:A:ARG:H    | 1:48:A:ARG:HD3  | 10       | 0.47          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 2        | 0.47          |
| (1,997)  | 1:34:A:MET:H    | 1:34:A:MET:HB2  | 5        | 0.47          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 8        | 0.47          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 12       | 0.47          |
| (1,487)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE21 | 3        | 0.47          |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 12       | 0.47          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 6        | 0.47          |
| (1,299)  | 1:10:A:GLN:HG2  | 1:11:A:ALA:HB2  | 1        | 0.47          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 4        | 0.47          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 6        | 0.47          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 7        | 0.47          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 10       | 0.47          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 11       | 0.47          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 13       | 0.47          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 14       | 0.47          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 15       | 0.47          |
| (1,26)   | 1:25:A:LEU:HB2  | 1:25:A:LEU:HD22 | 11       | 0.47          |
| (1,26)   | 1:25:A:LEU:HB2  | 1:25:A:LEU:HD22 | 15       | 0.47          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 2        | 0.46          |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 6        | 0.46          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 1        | 0.46          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 3        | 0.46          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 5        | 0.46          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 8        | 0.46          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 9        | 0.46          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 12       | 0.46          |
| (1,153)  | 1:49:A:THR:HG21 | 1:49:A:THR:HG1  | 13       | 0.46          |
| (1,26)   | 1:25:A:LEU:HB2  | 1:25:A:LEU:HD22 | 2        | 0.46          |
| (1,26)   | 1:25:A:LEU:HB2  | 1:25:A:LEU:HD22 | 3        | 0.46          |
| (1,26)   | 1:25:A:LEU:HB2  | 1:25:A:LEU:HD22 | 4        | 0.46          |
| (1,26)   | 1:25:A:LEU:HB2  | 1:25:A:LEU:HD22 | 8        | 0.46          |
| (1,26)   | 1:25:A:LEU:HB2  | 1:25:A:LEU:HD22 | 12       | 0.46          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 2        | 0.45          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 13       | 0.45          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 7        | 0.45          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 12       | 0.45          |
| (1,703)  | 1:7:A:PHE:H     | 1:7:A:PHE:HD2   | 10       | 0.45          |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 5        | 0.45          |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 11       | 0.45          |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 13       | 0.45          |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 6        | 0.45          |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 13       | 0.45          |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 5        | 0.45          |
| (1,471)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD22 | 4        | 0.45          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 12       | 0.45          |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 7        | 0.45          |
| (1,183)  | 1:54:A:THR:HA   | 1:54:A:THR:HG21 | 2        | 0.45          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 6        | 0.45          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 5        | 0.44          |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 5        | 0.44          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 4        | 0.44          |
| (1,657)  | 1:62:A:PRO:HG3  | 1:62:A:PRO:HD2  | 6        | 0.44          |
| (1,647)  | 1:60:A:VAL:HG22 | 1:10:A:GLN:H    | 11       | 0.44          |
| (1,519)  | 1:33:A:VAL:HG12 | 1:9:A:TYR:HE1   | 9        | 0.44          |
| (1,471)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD22 | 8        | 0.44          |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 9        | 0.44          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 4        | 0.44          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 6        | 0.44          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 7        | 0.44          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 8        | 0.44          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 7        | 0.44          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 8        | 0.44          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 10       | 0.44          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 1        | 0.43          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 1        | 0.43          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 2        | 0.43          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 13       | 0.43          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 10       | 0.43          |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 6        | 0.43          |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 8        | 0.43          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 3        | 0.43          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 6        | 0.43          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 9        | 0.43          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 12       | 0.43          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 15       | 0.43          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 7        | 0.42          |
| (1,831)  | 1:4:A:GLN:H     | 1:4:A:GLN:HG2   | 13       | 0.42          |
| (1,750)  | 1:19:A:ASN:H    | 1:18:A:GLN:HG2  | 14       | 0.42          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 2        | 0.42          |
| (1,471)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD22 | 11       | 0.42          |
| (1,471)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD22 | 15       | 0.42          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 11       | 0.42          |
| (1,299)  | 1:10:A:GLN:HG2  | 1:11:A:ALA:HB2  | 15       | 0.42          |
| (1,228)  | 1:65:A:LEU:HB2  | 1:65:A:LEU:HA   | 2        | 0.42          |
| (1,228)  | 1:65:A:LEU:HB2  | 1:65:A:LEU:HA   | 13       | 0.42          |
| (1,228)  | 1:65:A:LEU:HB2  | 1:65:A:LEU:HA   | 15       | 0.42          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 1        | 0.42          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 5        | 0.42          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 11       | 0.42          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 13       | 0.42          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 14       | 0.42          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 15       | 0.42          |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 10       | 0.41          |
| (1,750)  | 1:19:A:ASN:H    | 1:18:A:GLN:HG2  | 4        | 0.41          |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 10       | 0.41          |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 12       | 0.41          |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 2        | 0.41          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 10       | 0.41          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 5        | 0.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 13       | 0.41          |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 15       | 0.41          |
| (1,471)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD22 | 12       | 0.41          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 2        | 0.41          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 15       | 0.41          |
| (1,228)  | 1:65:A:LEU:HB2  | 1:65:A:LEU:HA   | 5        | 0.41          |
| (1,228)  | 1:65:A:LEU:HB2  | 1:65:A:LEU:HA   | 9        | 0.41          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 2        | 0.41          |
| (1,65)   | 1:34:A:MET:HG2  | 1:35:A:GLU:HB2  | 7        | 0.41          |
| (1,61)   | 1:34:A:MET:HB2  | 1:34:A:MET:HG2  | 11       | 0.41          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 5        | 0.4           |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 11       | 0.4           |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 15       | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 1        | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 2        | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 4        | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 7        | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 8        | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 9        | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 10       | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 11       | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 12       | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 14       | 0.4           |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 15       | 0.4           |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 1        | 0.4           |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 5        | 0.4           |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 8        | 0.4           |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 9        | 0.4           |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 11       | 0.4           |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 12       | 0.4           |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 13       | 0.4           |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 15       | 0.4           |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 8        | 0.4           |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 13       | 0.4           |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 6        | 0.4           |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 4        | 0.4           |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 13       | 0.4           |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 1        | 0.4           |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 9        | 0.4           |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 10       | 0.4           |
| (1,129)  | 1:45:A:THR:HB   | 1:32:A:ASP:HB2  | 7        | 0.4           |
| (1,61)   | 1:34:A:MET:HB2  | 1:34:A:MET:HG2  | 1        | 0.4           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,61)   | 1:34:A:MET:HB2  | 1:34:A:MET:HG2  | 2        | 0.4           |
| (1,61)   | 1:34:A:MET:HB2  | 1:34:A:MET:HG2  | 4        | 0.4           |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 2        | 0.4           |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 3        | 0.39          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 6        | 0.39          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 12       | 0.39          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 15       | 0.39          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 8        | 0.39          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 6        | 0.39          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 3        | 0.39          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 6        | 0.39          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 2        | 0.39          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 3        | 0.39          |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 5        | 0.39          |
| (1,664)  | 1:64:A:TYR:HB2  | 1:64:A:TYR:HE1  | 9        | 0.39          |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 3        | 0.39          |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 5        | 0.39          |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 6        | 0.39          |
| (1,659)  | 1:63:A:LEU:HB2  | 1:63:A:LEU:HA   | 13       | 0.39          |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 3        | 0.39          |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 4        | 0.39          |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 7        | 0.39          |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 10       | 0.39          |
| (1,656)  | 1:62:A:PRO:HG2  | 1:62:A:PRO:HD3  | 14       | 0.39          |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 5        | 0.39          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 15       | 0.39          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 15       | 0.39          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 4        | 0.39          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 9        | 0.39          |
| (1,471)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD22 | 3        | 0.39          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 13       | 0.39          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 14       | 0.39          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 3        | 0.39          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 12       | 0.39          |
| (1,61)   | 1:34:A:MET:HB2  | 1:34:A:MET:HG2  | 14       | 0.39          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 14       | 0.38          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 10       | 0.38          |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 4        | 0.38          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 14       | 0.38          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 8        | 0.38          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 3        | 0.38          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 7        | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 1        | 0.38          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 13       | 0.38          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 5        | 0.38          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 7        | 0.38          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 8        | 0.38          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 11       | 0.38          |
| (1,355)  | 1:52:A:PHE:HA   | 1:23:A:LEU:HD22 | 13       | 0.38          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 2        | 0.38          |
| (1,154)  | 1:49:A:THR:HG21 | 1:48:A:ARG:HB2  | 4        | 0.38          |
| (1,61)   | 1:34:A:MET:HB2  | 1:34:A:MET:HG2  | 5        | 0.38          |
| (1,61)   | 1:34:A:MET:HB2  | 1:34:A:MET:HG2  | 13       | 0.38          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 6        | 0.37          |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 6        | 0.37          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 6        | 0.37          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 11       | 0.37          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 2        | 0.37          |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 7        | 0.37          |
| (1,580)  | 1:50:A:LYS:HA   | 1:45:A:THR:HG21 | 2        | 0.37          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 6        | 0.37          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 2        | 0.37          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 13       | 0.37          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 5        | 0.37          |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 14       | 0.37          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 15       | 0.37          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 4        | 0.37          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 5        | 0.37          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 7        | 0.37          |
| (1,228)  | 1:65:A:LEU:HB2  | 1:65:A:LEU:HA   | 8        | 0.37          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 8        | 0.36          |
| (1,965)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB3  | 10       | 0.36          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 12       | 0.36          |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 7        | 0.36          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 9        | 0.36          |
| (1,661)  | 1:8:A:SER:HB3   | 1:63:A:LEU:HD12 | 11       | 0.36          |
| (1,532)  | 1:36:A:LYS:HD2  | 1:36:A:LYS:HA   | 6        | 0.36          |
| (1,532)  | 1:36:A:LYS:HD2  | 1:36:A:LYS:HA   | 11       | 0.36          |
| (1,532)  | 1:36:A:LYS:HD2  | 1:36:A:LYS:HA   | 15       | 0.36          |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 1        | 0.36          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 8        | 0.36          |
| (1,269)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG21 | 15       | 0.36          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 12       | 0.36          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 1        | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 5        | 0.36          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 14       | 0.36          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 9        | 0.35          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 11       | 0.35          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 1        | 0.35          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 12       | 0.35          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 3        | 0.35          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 12       | 0.35          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 1        | 0.35          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 10       | 0.35          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 14       | 0.35          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 6        | 0.35          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 14       | 0.35          |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 6        | 0.35          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 4        | 0.35          |
| (1,471)  | 1:25:A:LEU:HA   | 1:25:A:LEU:HD22 | 2        | 0.35          |
| (1,274)  | 1:8:A:SER:HB2   | 1:63:A:LEU:HB3  | 8        | 0.35          |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 15       | 0.35          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 9        | 0.35          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 7        | 0.35          |
| (1,65)   | 1:34:A:MET:HG2  | 1:35:A:GLU:HB2  | 9        | 0.35          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 2        | 0.34          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 7        | 0.34          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 6        | 0.34          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 1        | 0.34          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 11       | 0.34          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 14       | 0.34          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 8        | 0.34          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 10       | 0.34          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 10       | 0.34          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 14       | 0.34          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 11       | 0.34          |
| (1,532)  | 1:36:A:LYS:HD2  | 1:36:A:LYS:HA   | 1        | 0.34          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 11       | 0.34          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 3        | 0.34          |
| (1,274)  | 1:8:A:SER:HB2   | 1:63:A:LEU:HB3  | 2        | 0.34          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 2        | 0.34          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 3        | 0.34          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 5        | 0.34          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 6        | 0.34          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 8        | 0.34          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 14       | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 15       | 0.34          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 9        | 0.34          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 6        | 0.34          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 4        | 0.33          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 8        | 0.33          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 13       | 0.33          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 15       | 0.33          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 5        | 0.33          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 15       | 0.33          |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 4        | 0.33          |
| (1,532)  | 1:36:A:LYS:HD2  | 1:36:A:LYS:HA   | 13       | 0.33          |
| (1,501)  | 1:48:A:ARG:HA   | 1:48:A:ARG:HG2  | 4        | 0.33          |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 11       | 0.33          |
| (1,300)  | 1:10:A:GLN:HG2  | 1:61:A:LYS:HG3  | 14       | 0.33          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 3        | 0.33          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 1        | 0.33          |
| (1,147)  | 1:48:A:ARG:HG3  | 1:48:A:ARG:HD3  | 12       | 0.33          |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 4        | 0.33          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 5        | 0.32          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 10       | 0.32          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 14       | 0.32          |
| (1,965)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB3  | 12       | 0.32          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 2        | 0.32          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 3        | 0.32          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 5        | 0.32          |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 10       | 0.32          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 5        | 0.32          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 4        | 0.32          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 7        | 0.32          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 10       | 0.32          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 9        | 0.32          |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 2        | 0.32          |
| (1,274)  | 1:8:A:SER:HB2   | 1:63:A:LEU:HB3  | 1        | 0.32          |
| (1,274)  | 1:8:A:SER:HB2   | 1:63:A:LEU:HB3  | 7        | 0.32          |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 1        | 0.31          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 10       | 0.31          |
| (1,834)  | 1:5:A:ASP:HB2   | 1:5:A:ASP:H     | 13       | 0.31          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 9        | 0.31          |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 12       | 0.31          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 7        | 0.31          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 11       | 0.31          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 8        | 0.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,532)  | 1:36:A:LYS:HD2  | 1:36:A:LYS:HA   | 4        | 0.31          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 1        | 0.31          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 9        | 0.31          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 10       | 0.31          |
| (1,149)  | 1:49:A:THR:HA   | 1:49:A:THR:HG21 | 4        | 0.31          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 6        | 0.31          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 12       | 0.31          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 1        | 0.3           |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 4        | 0.3           |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 11       | 0.3           |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 15       | 0.3           |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 4        | 0.3           |
| (1,777)  | 1:23:A:LEU:H    | 1:54:A:THR:HG21 | 9        | 0.3           |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 2        | 0.3           |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 3        | 0.3           |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 11       | 0.3           |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 5        | 0.3           |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 2        | 0.3           |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 8        | 0.3           |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 15       | 0.3           |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 2        | 0.3           |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 12       | 0.3           |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 6        | 0.3           |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 9        | 0.3           |
| (1,274)  | 1:8:A:SER:HB2   | 1:63:A:LEU:HB3  | 13       | 0.3           |
| (1,274)  | 1:8:A:SER:HB2   | 1:63:A:LEU:HB3  | 15       | 0.3           |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 13       | 0.3           |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 12       | 0.3           |
| (1,117)  | 1:43:A:VAL:HG12 | 1:34:A:MET:HB2  | 13       | 0.3           |
| (1,103)  | 1:42:A:PHE:HB3  | 1:33:A:VAL:HG22 | 2        | 0.3           |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 7        | 0.29          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 12       | 0.29          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 10       | 0.29          |
| (1,580)  | 1:50:A:LYS:HA   | 1:45:A:THR:HG21 | 1        | 0.29          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 6        | 0.29          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 12       | 0.29          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 9        | 0.29          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 5        | 0.29          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 6        | 0.29          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 13       | 0.29          |
| (1,150)  | 1:49:A:THR:HA   | 1:48:A:ARG:HG3  | 6        | 0.29          |
| (1,1159) | 1:65:A:LEU:H    | 1:65:A:LEU:HB2  | 1        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 15       | 0.28          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 15       | 0.28          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 2        | 0.28          |
| (1,802)  | 1:32:A:ASP:H    | 1:31:A:VAL:HG22 | 5        | 0.28          |
| (1,679)  | 1:33:A:VAL:H    | 1:32:A:ASP:HB2  | 5        | 0.28          |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 14       | 0.28          |
| (1,580)  | 1:50:A:LYS:HA   | 1:45:A:THR:HG21 | 13       | 0.28          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 9        | 0.28          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 15       | 0.28          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 14       | 0.28          |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 11       | 0.28          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 10       | 0.28          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 14       | 0.28          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 3        | 0.28          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 3        | 0.28          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 14       | 0.28          |
| (1,1159) | 1:65:A:LEU:H    | 1:65:A:LEU:HB2  | 12       | 0.27          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 3        | 0.27          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 5        | 0.27          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 9        | 0.27          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 12       | 0.27          |
| (1,1048) | 1:46:A:SER:H    | 1:45:A:THR:HG21 | 13       | 0.27          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 6        | 0.27          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 9        | 0.27          |
| (1,545)  | 1:44:A:GLY:HA3  | 1:34:A:MET:HB2  | 10       | 0.27          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 12       | 0.27          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 13       | 0.27          |
| (1,501)  | 1:48:A:ARG:HA   | 1:48:A:ARG:HG2  | 12       | 0.27          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 7        | 0.27          |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 10       | 0.27          |
| (1,269)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 3        | 0.27          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 8        | 0.27          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 2        | 0.27          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 5        | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 4        | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 5        | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 6        | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 7        | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 8        | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 9        | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 10       | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 11       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 12       | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 13       | 0.27          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 15       | 0.27          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 1        | 0.26          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 4        | 0.26          |
| (1,1015) | 1:36:A:LYS:H    | 1:35:A:GLU:HG2  | 5        | 0.26          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 13       | 0.26          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 12       | 0.26          |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 3        | 0.26          |
| (1,487)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE21 | 7        | 0.26          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 3        | 0.26          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 1        | 0.26          |
| (1,269)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG23 | 1        | 0.26          |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 15       | 0.26          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 1        | 0.26          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 5        | 0.26          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 1        | 0.26          |
| (1,1)    | 1:22:A:GLU:HA   | 1:22:A:GLU:HB2  | 2        | 0.26          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 6        | 0.25          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 13       | 0.25          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 3        | 0.25          |
| (1,1002) | 1:35:A:GLU:H    | 1:35:A:GLU:HB2  | 13       | 0.25          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 4        | 0.25          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 8        | 0.25          |
| (1,845)  | 1:7:A:PHE:H     | 1:6:A:LEU:HD21  | 6        | 0.25          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 3        | 0.25          |
| (1,580)  | 1:50:A:LYS:HA   | 1:45:A:THR:HG21 | 6        | 0.25          |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 3        | 0.25          |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 4        | 0.25          |
| (1,255)  | 1:6:A:LEU:HD22  | 1:6:A:LEU:HA    | 12       | 0.25          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 3        | 0.25          |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 8        | 0.25          |
| (1,1159) | 1:65:A:LEU:H    | 1:65:A:LEU:HB2  | 6        | 0.24          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 11       | 0.24          |
| (1,1112) | 1:55:A:PHE:H    | 1:42:A:PHE:HB3  | 7        | 0.24          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 9        | 0.24          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 5        | 0.24          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 12       | 0.24          |
| (1,785)  | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 12       | 0.24          |
| (1,750)  | 1:19:A:ASN:H    | 1:18:A:GLN:HG2  | 12       | 0.24          |
| (1,580)  | 1:50:A:LYS:HA   | 1:45:A:THR:HG21 | 14       | 0.24          |
| (1,534)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HD1  | 13       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 6        | 0.24          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 9        | 0.24          |
| (1,528)  | 1:35:A:GLU:HB2  | 1:36:A:LYS:H    | 10       | 0.24          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 2        | 0.24          |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 10       | 0.24          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 3        | 0.24          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 4        | 0.24          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 9        | 0.24          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 7        | 0.24          |
| (1,45)   | 1:21:A:ASP:HB2  | 1:21:A:ASP:HA   | 10       | 0.24          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 2        | 0.23          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 10       | 0.23          |
| (1,1089) | 1:50:A:LYS:H    | 1:45:A:THR:HG23 | 8        | 0.23          |
| (1,1015) | 1:36:A:LYS:H    | 1:35:A:GLU:HG2  | 4        | 0.23          |
| (1,994)  | 1:34:A:MET:H    | 1:44:A:GLY:HA3  | 2        | 0.23          |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 7        | 0.23          |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 13       | 0.23          |
| (1,965)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB3  | 6        | 0.23          |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 3        | 0.23          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 3        | 0.23          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 4        | 0.23          |
| (1,873)  | 1:18:A:GLN:H    | 1:15:A:TYR:HE1  | 8        | 0.23          |
| (1,785)  | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 5        | 0.23          |
| (1,679)  | 1:33:A:VAL:H    | 1:32:A:ASP:HB2  | 9        | 0.23          |
| (1,667)  | 1:10:A:GLN:HB2  | 1:61:A:LYS:HG3  | 13       | 0.23          |
| (1,626)  | 1:57:A:GLY:HA3  | 1:60:A:VAL:HG22 | 2        | 0.23          |
| (1,596)  | 1:22:A:GLU:HG2  | 1:54:A:THR:HG21 | 13       | 0.23          |
| (1,549)  | 1:45:A:THR:HG21 | 1:45:A:THR:HG1  | 5        | 0.23          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 2        | 0.23          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 12       | 0.23          |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 1        | 0.23          |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 4        | 0.23          |
| (1,274)  | 1:8:A:SER:HB2   | 1:63:A:LEU:HB3  | 3        | 0.23          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 1        | 0.23          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 7        | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 1        | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 2        | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 5        | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 6        | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 7        | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 8        | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3  | 1:51:A:GLN:HB3  | 10       | 0.23          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,161)  | 1:51:A:GLN:HG3 | 1:51:A:GLN:HB3  | 11       | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3 | 1:51:A:GLN:HB3  | 12       | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3 | 1:51:A:GLN:HB3  | 13       | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3 | 1:51:A:GLN:HB3  | 14       | 0.23          |
| (1,161)  | 1:51:A:GLN:HG3 | 1:51:A:GLN:HB3  | 15       | 0.23          |
| (1,127)  | 1:45:A:THR:HA  | 1:31:A:VAL:HG23 | 8        | 0.23          |
| (1,127)  | 1:45:A:THR:HA  | 1:31:A:VAL:HG23 | 15       | 0.23          |
| (1,45)   | 1:21:A:ASP:HB2 | 1:21:A:ASP:HA   | 4        | 0.23          |
| (1,45)   | 1:21:A:ASP:HB2 | 1:21:A:ASP:HA   | 13       | 0.23          |
| (1,45)   | 1:21:A:ASP:HB2 | 1:21:A:ASP:HA   | 15       | 0.23          |
| (1,1153) | 1:64:A:TYR:H   | 1:63:A:LEU:HB3  | 5        | 0.22          |
| (1,1112) | 1:55:A:PHE:H   | 1:42:A:PHE:HB3  | 4        | 0.22          |
| (1,1112) | 1:55:A:PHE:H   | 1:42:A:PHE:HB3  | 14       | 0.22          |
| (1,1089) | 1:50:A:LYS:H   | 1:45:A:THR:HG23 | 7        | 0.22          |
| (1,994)  | 1:34:A:MET:H   | 1:44:A:GLY:HA3  | 1        | 0.22          |
| (1,992)  | 1:33:A:VAL:H   | 1:33:A:VAL:HG22 | 2        | 0.22          |
| (1,831)  | 1:4:A:GLN:H    | 1:4:A:GLN:HG2   | 14       | 0.22          |
| (1,802)  | 1:32:A:ASP:H   | 1:31:A:VAL:HG22 | 7        | 0.22          |
| (1,785)  | 1:25:A:LEU:H   | 1:24:A:GLU:HG2  | 3        | 0.22          |
| (1,700)  | 1:5:A:ASP:HB2  | 1:6:A:LEU:H     | 12       | 0.22          |
| (1,679)  | 1:33:A:VAL:H   | 1:32:A:ASP:HB2  | 7        | 0.22          |
| (1,580)  | 1:50:A:LYS:HA  | 1:45:A:THR:HG21 | 5        | 0.22          |
| (1,580)  | 1:50:A:LYS:HA  | 1:45:A:THR:HG21 | 11       | 0.22          |
| (1,531)  | 1:36:A:LYS:HB2 | 1:42:A:PHE:HE1  | 7        | 0.22          |
| (1,528)  | 1:35:A:GLU:HB2 | 1:36:A:LYS:H    | 11       | 0.22          |
| (1,511)  | 1:33:A:VAL:HA  | 1:44:A:GLY:HA3  | 12       | 0.22          |
| (1,358)  | 1:52:A:PHE:HA  | 1:52:A:PHE:HD2  | 2        | 0.22          |
| (1,358)  | 1:52:A:PHE:HA  | 1:52:A:PHE:HD2  | 6        | 0.22          |
| (1,358)  | 1:52:A:PHE:HA  | 1:52:A:PHE:HD2  | 7        | 0.22          |
| (1,358)  | 1:52:A:PHE:HA  | 1:52:A:PHE:HD2  | 8        | 0.22          |
| (1,358)  | 1:52:A:PHE:HA  | 1:52:A:PHE:HD2  | 12       | 0.22          |
| (1,358)  | 1:52:A:PHE:HA  | 1:52:A:PHE:HD2  | 15       | 0.22          |
| (1,269)  | 1:8:A:SER:HB2  | 1:30:A:ILE:HG21 | 7        | 0.22          |
| (1,240)  | 1:3:A:SER:HA   | 1:3:A:SER:HB2   | 5        | 0.22          |
| (1,240)  | 1:3:A:SER:HA   | 1:3:A:SER:HB2   | 6        | 0.22          |
| (1,37)   | 1:28:A:GLY:HA3 | 1:10:A:GLN:HG2  | 9        | 0.22          |
| (1,1130) | 1:60:A:VAL:H   | 1:59:A:TYR:HB3  | 8        | 0.21          |
| (1,1112) | 1:55:A:PHE:H   | 1:42:A:PHE:HB3  | 8        | 0.21          |
| (1,992)  | 1:33:A:VAL:H   | 1:33:A:VAL:HG22 | 1        | 0.21          |
| (1,992)  | 1:33:A:VAL:H   | 1:33:A:VAL:HG22 | 4        | 0.21          |
| (1,992)  | 1:33:A:VAL:H   | 1:33:A:VAL:HG22 | 11       | 0.21          |
| (1,785)  | 1:25:A:LEU:H   | 1:24:A:GLU:HG2  | 10       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,569)  | 1:48:A:ARG:HB3  | 1:49:A:THR:HG23 | 4        | 0.21          |
| (1,531)  | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 11       | 0.21          |
| (1,528)  | 1:35:A:GLU:HB2  | 1:36:A:LYS:H    | 2        | 0.21          |
| (1,511)  | 1:33:A:VAL:HA   | 1:44:A:GLY:HA3  | 5        | 0.21          |
| (1,501)  | 1:48:A:ARG:HA   | 1:48:A:ARG:HG2  | 3        | 0.21          |
| (1,501)  | 1:48:A:ARG:HA   | 1:48:A:ARG:HG2  | 6        | 0.21          |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 11       | 0.21          |
| (1,356)  | 1:52:A:PHE:HA   | 1:45:A:THR:HG21 | 4        | 0.21          |
| (1,356)  | 1:52:A:PHE:HA   | 1:45:A:THR:HG21 | 10       | 0.21          |
| (1,356)  | 1:52:A:PHE:HA   | 1:45:A:THR:HG21 | 14       | 0.21          |
| (1,240)  | 1:3:A:SER:HA    | 1:3:A:SER:HB2   | 2        | 0.21          |
| (1,240)  | 1:3:A:SER:HA    | 1:3:A:SER:HB2   | 3        | 0.21          |
| (1,240)  | 1:3:A:SER:HA    | 1:3:A:SER:HB2   | 4        | 0.21          |
| (1,240)  | 1:3:A:SER:HA    | 1:3:A:SER:HB2   | 8        | 0.21          |
| (1,240)  | 1:3:A:SER:HA    | 1:3:A:SER:HB2   | 15       | 0.21          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 2        | 0.21          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 9        | 0.21          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 11       | 0.21          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 4        | 0.21          |
| (1,63)   | 1:34:A:MET:HB2  | 1:34:A:MET:HE2  | 7        | 0.21          |
| (1,45)   | 1:21:A:ASP:HB2  | 1:21:A:ASP:HA   | 8        | 0.21          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 3        | 0.21          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 3        | 0.21          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 15       | 0.21          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 6        | 0.2           |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 8        | 0.2           |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 10       | 0.2           |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 12       | 0.2           |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 14       | 0.2           |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 1        | 0.2           |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 12       | 0.2           |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 15       | 0.2           |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 4        | 0.2           |
| (1,568)  | 1:48:A:ARG:HB2  | 1:49:A:THR:HG23 | 1        | 0.2           |
| (1,528)  | 1:35:A:GLU:HB2  | 1:36:A:LYS:H    | 6        | 0.2           |
| (1,518)  | 1:33:A:VAL:HB   | 1:7:A:PHE:HB3   | 11       | 0.2           |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 12       | 0.2           |
| (1,426)  | 1:46:A:SER:HA   | 1:31:A:VAL:HG22 | 14       | 0.2           |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 5        | 0.2           |
| (1,358)  | 1:52:A:PHE:HA   | 1:52:A:PHE:HD2  | 13       | 0.2           |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 5        | 0.2           |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 8        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 13       | 0.2           |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 15       | 0.2           |
| (1,142)  | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 15       | 0.2           |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 3        | 0.2           |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 9        | 0.2           |
| (1,1159) | 1:65:A:LEU:H    | 1:65:A:LEU:HB2  | 7        | 0.19          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 4        | 0.19          |
| (1,1112) | 1:55:A:PHE:H    | 1:42:A:PHE:HB3  | 6        | 0.19          |
| (1,994)  | 1:34:A:MET:H    | 1:44:A:GLY:HA3  | 13       | 0.19          |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 5        | 0.19          |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 6        | 0.19          |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 9        | 0.19          |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 15       | 0.19          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 7        | 0.19          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 10       | 0.19          |
| (1,866)  | 1:12:A:LEU:H    | 1:12:A:LEU:HD22 | 14       | 0.19          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 1        | 0.19          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 10       | 0.19          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 11       | 0.19          |
| (1,679)  | 1:33:A:VAL:H    | 1:32:A:ASP:HB2  | 14       | 0.19          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 2        | 0.19          |
| (1,564)  | 1:47:A:ARG:HG2  | 1:47:A:ARG:HA   | 5        | 0.19          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 7        | 0.19          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 8        | 0.19          |
| (1,518)  | 1:33:A:VAL:HB   | 1:7:A:PHE:HB3   | 6        | 0.19          |
| (1,454)  | 1:51:A:GLN:HG3  | 1:23:A:LEU:HD22 | 12       | 0.19          |
| (1,269)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG23 | 8        | 0.19          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 1        | 0.19          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 4        | 0.19          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 7        | 0.19          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 9        | 0.19          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 10       | 0.19          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 11       | 0.19          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 12       | 0.19          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 14       | 0.19          |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 10       | 0.19          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 13       | 0.19          |
| (1,103)  | 1:42:A:PHE:HB3  | 1:33:A:VAL:HG22 | 9        | 0.19          |
| (1,83)   | 1:38:A:ASP:HA   | 1:38:A:ASP:HB2  | 12       | 0.19          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 14       | 0.19          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 4        | 0.18          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 9        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 10       | 0.18          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 13       | 0.18          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 1        | 0.18          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 13       | 0.18          |
| (1,1112) | 1:55:A:PHE:H    | 1:42:A:PHE:HB3  | 11       | 0.18          |
| (1,1026) | 1:37:A:CYS:H    | 1:36:A:LYS:HB2  | 5        | 0.18          |
| (1,992)  | 1:33:A:VAL:H    | 1:33:A:VAL:HG22 | 3        | 0.18          |
| (1,953)  | 1:26:A:ARG:H    | 1:15:A:TYR:H    | 6        | 0.18          |
| (1,943)  | 1:25:A:LEU:H    | 1:15:A:TYR:HB2  | 9        | 0.18          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 6        | 0.18          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 11       | 0.18          |
| (1,860)  | 1:29:A:ASP:H    | 1:10:A:GLN:HG2  | 13       | 0.18          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 5        | 0.18          |
| (1,703)  | 1:7:A:PHE:H     | 1:7:A:PHE:HD2   | 3        | 0.18          |
| (1,700)  | 1:5:A:ASP:HB2   | 1:6:A:LEU:H     | 2        | 0.18          |
| (1,576)  | 1:49:A:THR:HB   | 1:46:A:SER:HB2  | 4        | 0.18          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 3        | 0.18          |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 15       | 0.18          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 4        | 0.18          |
| (1,223)  | 1:62:A:PRO:HA   | 1:62:A:PRO:HB2  | 3        | 0.18          |
| (1,142)  | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 6        | 0.18          |
| (1,142)  | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 14       | 0.18          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 10       | 0.18          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 11       | 0.18          |
| (1,83)   | 1:38:A:ASP:HA   | 1:38:A:ASP:HB2  | 9        | 0.18          |
| (1,83)   | 1:38:A:ASP:HA   | 1:38:A:ASP:HB2  | 10       | 0.18          |
| (1,1130) | 1:60:A:VAL:H    | 1:59:A:TYR:HB3  | 14       | 0.17          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 3        | 0.17          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 15       | 0.17          |
| (1,1112) | 1:55:A:PHE:H    | 1:42:A:PHE:HB3  | 10       | 0.17          |
| (1,1062) | 1:48:A:ARG:H    | 1:47:A:ARG:HB2  | 7        | 0.17          |
| (1,994)  | 1:34:A:MET:H    | 1:44:A:GLY:HA3  | 3        | 0.17          |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 11       | 0.17          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 9        | 0.17          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 7        | 0.17          |
| (1,785)  | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 7        | 0.17          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 8        | 0.17          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 14       | 0.17          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 15       | 0.17          |
| (1,762)  | 1:21:A:ASP:H    | 1:21:A:ASP:HB3  | 10       | 0.17          |
| (1,762)  | 1:21:A:ASP:H    | 1:21:A:ASP:HB3  | 15       | 0.17          |
| (1,700)  | 1:5:A:ASP:HB2   | 1:6:A:LEU:H     | 6        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,528)  | 1:35:A:GLU:HB2  | 1:36:A:LYS:H    | 14       | 0.17          |
| (1,356)  | 1:52:A:PHE:HA   | 1:45:A:THR:HG21 | 12       | 0.17          |
| (1,171)  | 1:45:A:THR:HG21 | 1:52:A:PHE:HB2  | 15       | 0.17          |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 4        | 0.17          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 8        | 0.17          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 1        | 0.16          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 7        | 0.16          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 12       | 0.16          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 15       | 0.16          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 6        | 0.16          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 11       | 0.16          |
| (1,1066) | 1:49:A:THR:H    | 1:49:A:THR:HG21 | 6        | 0.16          |
| (1,1062) | 1:48:A:ARG:H    | 1:47:A:ARG:HB2  | 1        | 0.16          |
| (1,1062) | 1:48:A:ARG:H    | 1:47:A:ARG:HB2  | 2        | 0.16          |
| (1,1026) | 1:37:A:CYS:H    | 1:36:A:LYS:HB2  | 7        | 0.16          |
| (1,994)  | 1:34:A:MET:H    | 1:44:A:GLY:HA3  | 8        | 0.16          |
| (1,890)  | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 13       | 0.16          |
| (1,845)  | 1:7:A:PHE:H     | 1:6:A:LEU:HD21  | 5        | 0.16          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 15       | 0.16          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 4        | 0.16          |
| (1,793)  | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 11       | 0.16          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 2        | 0.16          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 6        | 0.16          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 7        | 0.16          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 9        | 0.16          |
| (1,762)  | 1:21:A:ASP:H    | 1:21:A:ASP:HB3  | 4        | 0.16          |
| (1,762)  | 1:21:A:ASP:H    | 1:21:A:ASP:HB3  | 13       | 0.16          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 10       | 0.16          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 13       | 0.16          |
| (1,580)  | 1:50:A:LYS:HA   | 1:45:A:THR:HG21 | 12       | 0.16          |
| (1,570)  | 1:48:A:ARG:HB2  | 1:49:A:THR:H    | 4        | 0.16          |
| (1,557)  | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 3        | 0.16          |
| (1,548)  | 1:45:A:THR:HG21 | 1:50:A:LYS:H    | 9        | 0.16          |
| (1,538)  | 1:37:A:CYS:HB2  | 1:40:A:GLY:H    | 3        | 0.16          |
| (1,501)  | 1:48:A:ARG:HA   | 1:48:A:ARG:HG2  | 10       | 0.16          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 1        | 0.16          |
| (1,495)  | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 1        | 0.16          |
| (1,458)  | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 12       | 0.16          |
| (1,405)  | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 6        | 0.16          |
| (1,405)  | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 10       | 0.16          |
| (1,356)  | 1:52:A:PHE:HA   | 1:45:A:THR:HG21 | 13       | 0.16          |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 7        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,97)   | 1:42:A:PHE:HA   | 1:42:A:PHE:HB2  | 13       | 0.16          |
| (1,63)   | 1:34:A:MET:HB2  | 1:34:A:MET:HE2  | 9        | 0.16          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 5        | 0.15          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 7        | 0.15          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 9        | 0.15          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 12       | 0.15          |
| (1,1059) | 1:48:A:ARG:H    | 1:48:A:ARG:HG2  | 4        | 0.15          |
| (1,1011) | 1:36:A:LYS:H    | 1:33:A:VAL:HG22 | 4        | 0.15          |
| (1,958)  | 1:27:A:ASP:H    | 1:14:A:SER:HB3  | 9        | 0.15          |
| (1,911)  | 1:42:A:PHE:H    | 1:41:A:TRP:HB2  | 9        | 0.15          |
| (1,899)  | 1:31:A:VAL:H    | 1:30:A:ILE:HG13 | 15       | 0.15          |
| (1,785)  | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 2        | 0.15          |
| (1,785)  | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 15       | 0.15          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 3        | 0.15          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 12       | 0.15          |
| (1,771)  | 1:22:A:GLU:H    | 1:22:A:GLU:HB3  | 13       | 0.15          |
| (1,704)  | 1:6:A:LEU:H     | 1:7:A:PHE:H     | 7        | 0.15          |
| (1,700)  | 1:5:A:ASP:HB2   | 1:6:A:LEU:H     | 13       | 0.15          |
| (1,679)  | 1:33:A:VAL:H    | 1:32:A:ASP:HB2  | 10       | 0.15          |
| (1,676)  | 1:11:A:ALA:H    | 1:10:A:GLN:HB3  | 13       | 0.15          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 6        | 0.15          |
| (1,568)  | 1:48:A:ARG:HB2  | 1:49:A:THR:HG23 | 8        | 0.15          |
| (1,557)  | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 2        | 0.15          |
| (1,557)  | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 4        | 0.15          |
| (1,556)  | 1:46:A:SER:HB2  | 1:23:A:LEU:HD22 | 1        | 0.15          |
| (1,538)  | 1:37:A:CYS:HB2  | 1:40:A:GLY:H    | 1        | 0.15          |
| (1,528)  | 1:35:A:GLU:HB2  | 1:36:A:LYS:H    | 3        | 0.15          |
| (1,528)  | 1:35:A:GLU:HB2  | 1:36:A:LYS:H    | 4        | 0.15          |
| (1,405)  | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 12       | 0.15          |
| (1,405)  | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 13       | 0.15          |
| (1,338)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 1        | 0.15          |
| (1,330)  | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 4        | 0.15          |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 11       | 0.15          |
| (1,142)  | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 11       | 0.15          |
| (1,142)  | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 12       | 0.15          |
| (1,127)  | 1:45:A:THR:HA   | 1:31:A:VAL:HG23 | 14       | 0.15          |
| (1,97)   | 1:42:A:PHE:HA   | 1:42:A:PHE:HB2  | 1        | 0.15          |
| (1,97)   | 1:42:A:PHE:HA   | 1:42:A:PHE:HB2  | 2        | 0.15          |
| (1,97)   | 1:42:A:PHE:HA   | 1:42:A:PHE:HB2  | 3        | 0.15          |
| (1,97)   | 1:42:A:PHE:HA   | 1:42:A:PHE:HB2  | 4        | 0.15          |
| (1,97)   | 1:42:A:PHE:HA   | 1:42:A:PHE:HB2  | 5        | 0.15          |
| (1,97)   | 1:42:A:PHE:HA   | 1:42:A:PHE:HB2  | 6        | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,97)   | 1:42:A:PHE:HA  | 1:42:A:PHE:HB2  | 7        | 0.15          |
| (1,97)   | 1:42:A:PHE:HA  | 1:42:A:PHE:HB2  | 8        | 0.15          |
| (1,97)   | 1:42:A:PHE:HA  | 1:42:A:PHE:HB2  | 9        | 0.15          |
| (1,97)   | 1:42:A:PHE:HA  | 1:42:A:PHE:HB2  | 10       | 0.15          |
| (1,97)   | 1:42:A:PHE:HA  | 1:42:A:PHE:HB2  | 11       | 0.15          |
| (1,97)   | 1:42:A:PHE:HA  | 1:42:A:PHE:HB2  | 12       | 0.15          |
| (1,97)   | 1:42:A:PHE:HA  | 1:42:A:PHE:HB2  | 14       | 0.15          |
| (1,97)   | 1:42:A:PHE:HA  | 1:42:A:PHE:HB2  | 15       | 0.15          |
| (1,1153) | 1:64:A:TYR:H   | 1:63:A:LEU:HB3  | 2        | 0.14          |
| (1,1124) | 1:59:A:TYR:H   | 1:59:A:TYR:HB3  | 10       | 0.14          |
| (1,1112) | 1:55:A:PHE:H   | 1:42:A:PHE:HB3  | 5        | 0.14          |
| (1,1026) | 1:37:A:CYS:H   | 1:36:A:LYS:HB2  | 2        | 0.14          |
| (1,1026) | 1:37:A:CYS:H   | 1:36:A:LYS:HB2  | 3        | 0.14          |
| (1,994)  | 1:34:A:MET:H   | 1:44:A:GLY:HA3  | 6        | 0.14          |
| (1,965)  | 1:27:A:ASP:H   | 1:26:A:ARG:HB3  | 8        | 0.14          |
| (1,911)  | 1:42:A:PHE:H   | 1:41:A:TRP:HB2  | 15       | 0.14          |
| (1,835)  | 1:5:A:ASP:H    | 1:4:A:GLN:HG2   | 1        | 0.14          |
| (1,835)  | 1:5:A:ASP:H    | 1:4:A:GLN:HG2   | 2        | 0.14          |
| (1,785)  | 1:25:A:LEU:H   | 1:24:A:GLU:HG2  | 6        | 0.14          |
| (1,785)  | 1:25:A:LEU:H   | 1:24:A:GLU:HG2  | 8        | 0.14          |
| (1,771)  | 1:22:A:GLU:H   | 1:22:A:GLU:HB3  | 1        | 0.14          |
| (1,676)  | 1:11:A:ALA:H   | 1:10:A:GLN:HB3  | 4        | 0.14          |
| (1,596)  | 1:22:A:GLU:HG2 | 1:54:A:THR:HG21 | 4        | 0.14          |
| (1,568)  | 1:48:A:ARG:HB2 | 1:49:A:THR:HG23 | 2        | 0.14          |
| (1,568)  | 1:48:A:ARG:HB2 | 1:49:A:THR:HG23 | 3        | 0.14          |
| (1,568)  | 1:48:A:ARG:HB2 | 1:49:A:THR:HG23 | 7        | 0.14          |
| (1,568)  | 1:48:A:ARG:HB2 | 1:49:A:THR:HG23 | 13       | 0.14          |
| (1,557)  | 1:23:A:LEU:HG  | 1:46:A:SER:HB2  | 5        | 0.14          |
| (1,538)  | 1:37:A:CYS:HB2 | 1:40:A:GLY:H    | 13       | 0.14          |
| (1,528)  | 1:35:A:GLU:HB2 | 1:36:A:LYS:H    | 5        | 0.14          |
| (1,528)  | 1:35:A:GLU:HB2 | 1:36:A:LYS:H    | 7        | 0.14          |
| (1,475)  | 1:26:A:ARG:HB2 | 1:26:A:ARG:HD2  | 5        | 0.14          |
| (1,458)  | 1:25:A:LEU:HB2 | 1:15:A:TYR:HB3  | 9        | 0.14          |
| (1,358)  | 1:52:A:PHE:HA  | 1:52:A:PHE:HD2  | 14       | 0.14          |
| (1,356)  | 1:52:A:PHE:HA  | 1:45:A:THR:HG21 | 2        | 0.14          |
| (1,209)  | 1:61:A:LYS:HB3 | 1:61:A:LYS:HA   | 9        | 0.14          |
| (1,87)   | 1:39:A:ASP:HB3 | 1:39:A:ASP:H    | 9        | 0.14          |
| (1,12)   | 1:35:A:GLU:HA  | 1:36:A:LYS:HG2  | 15       | 0.14          |
| (1,1154) | 1:64:A:TYR:H   | 1:63:A:LEU:HD12 | 8        | 0.13          |
| (1,1112) | 1:55:A:PHE:H   | 1:42:A:PHE:HB3  | 2        | 0.13          |
| (1,1112) | 1:55:A:PHE:H   | 1:42:A:PHE:HB3  | 9        | 0.13          |
| (1,1011) | 1:36:A:LYS:H   | 1:33:A:VAL:HG22 | 13       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,965)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB3  | 9        | 0.13          |
| (1,964)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB2  | 13       | 0.13          |
| (1,916)  | 1:40:A:GLY:H    | 1:42:A:PHE:HD1  | 13       | 0.13          |
| (1,899)  | 1:31:A:VAL:H    | 1:30:A:ILE:HG13 | 1        | 0.13          |
| (1,835)  | 1:5:A:ASP:H     | 1:4:A:GLN:HG2   | 11       | 0.13          |
| (1,829)  | 1:4:A:GLN:H     | 1:3:A:SER:HA    | 1        | 0.13          |
| (1,768)  | 1:21:A:ASP:H    | 1:22:A:GLU:H    | 3        | 0.13          |
| (1,700)  | 1:5:A:ASP:HB2   | 1:6:A:LEU:H     | 14       | 0.13          |
| (1,679)  | 1:33:A:VAL:H    | 1:32:A:ASP:HB2  | 2        | 0.13          |
| (1,660)  | 1:6:A:LEU:HB2   | 1:5:A:ASP:H     | 7        | 0.13          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 1        | 0.13          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 7        | 0.13          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 15       | 0.13          |
| (1,557)  | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 9        | 0.13          |
| (1,538)  | 1:37:A:CYS:HB2  | 1:40:A:GLY:H    | 8        | 0.13          |
| (1,532)  | 1:36:A:LYS:HD2  | 1:36:A:LYS:HA   | 5        | 0.13          |
| (1,528)  | 1:35:A:GLU:HB2  | 1:36:A:LYS:H    | 8        | 0.13          |
| (1,509)  | 1:32:A:ASP:HB2  | 1:45:A:THR:HG23 | 6        | 0.13          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 8        | 0.13          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 15       | 0.13          |
| (1,484)  | 1:30:A:ILE:HD12 | 1:30:A:ILE:HA   | 5        | 0.13          |
| (1,405)  | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 2        | 0.13          |
| (1,405)  | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 9        | 0.13          |
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 15       | 0.13          |
| (1,338)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 5        | 0.13          |
| (1,330)  | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 3        | 0.13          |
| (1,330)  | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 5        | 0.13          |
| (1,330)  | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 15       | 0.13          |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 6        | 0.13          |
| (1,87)   | 1:39:A:ASP:HB3  | 1:39:A:ASP:H    | 10       | 0.13          |
| (1,79)   | 1:37:A:CYS:HA   | 1:37:A:CYS:HB3  | 4        | 0.13          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 11       | 0.13          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 14       | 0.13          |
| (1,1154) | 1:64:A:TYR:H    | 1:63:A:LEU:HD12 | 7        | 0.12          |
| (1,1154) | 1:64:A:TYR:H    | 1:63:A:LEU:HD12 | 11       | 0.12          |
| (1,1154) | 1:64:A:TYR:H    | 1:63:A:LEU:HD12 | 13       | 0.12          |
| (1,1153) | 1:64:A:TYR:H    | 1:63:A:LEU:HB3  | 8        | 0.12          |
| (1,1062) | 1:48:A:ARG:H    | 1:47:A:ARG:HB2  | 8        | 0.12          |
| (1,994)  | 1:34:A:MET:H    | 1:44:A:GLY:HA3  | 12       | 0.12          |
| (1,994)  | 1:34:A:MET:H    | 1:44:A:GLY:HA3  | 15       | 0.12          |
| (1,964)  | 1:27:A:ASP:H    | 1:26:A:ARG:HB2  | 7        | 0.12          |
| (1,953)  | 1:26:A:ARG:H    | 1:15:A:TYR:H    | 4        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,943) | 1:25:A:LEU:H    | 1:15:A:TYR:HB2  | 3        | 0.12          |
| (1,943) | 1:25:A:LEU:H    | 1:15:A:TYR:HB2  | 14       | 0.12          |
| (1,943) | 1:25:A:LEU:H    | 1:15:A:TYR:HB2  | 15       | 0.12          |
| (1,916) | 1:40:A:GLY:H    | 1:42:A:PHE:HD1  | 2        | 0.12          |
| (1,899) | 1:31:A:VAL:H    | 1:30:A:ILE:HG13 | 13       | 0.12          |
| (1,884) | 1:54:A:THR:H    | 1:54:A:THR:HG1  | 14       | 0.12          |
| (1,785) | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 9        | 0.12          |
| (1,785) | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 11       | 0.12          |
| (1,785) | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 14       | 0.12          |
| (1,769) | 1:22:A:GLU:H    | 1:21:A:ASP:HB3  | 2        | 0.12          |
| (1,762) | 1:21:A:ASP:H    | 1:21:A:ASP:HB3  | 8        | 0.12          |
| (1,700) | 1:5:A:ASP:HB2   | 1:6:A:LEU:H     | 4        | 0.12          |
| (1,679) | 1:33:A:VAL:H    | 1:32:A:ASP:HB2  | 13       | 0.12          |
| (1,629) | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 3        | 0.12          |
| (1,629) | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 5        | 0.12          |
| (1,629) | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 11       | 0.12          |
| (1,629) | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 12       | 0.12          |
| (1,568) | 1:48:A:ARG:HB2  | 1:49:A:THR:HG23 | 10       | 0.12          |
| (1,568) | 1:48:A:ARG:HB2  | 1:49:A:THR:HG23 | 15       | 0.12          |
| (1,538) | 1:37:A:CYS:HB2  | 1:40:A:GLY:H    | 14       | 0.12          |
| (1,538) | 1:37:A:CYS:HB2  | 1:40:A:GLY:H    | 15       | 0.12          |
| (1,531) | 1:36:A:LYS:HB2  | 1:42:A:PHE:HE1  | 15       | 0.12          |
| (1,518) | 1:33:A:VAL:HB   | 1:7:A:PHE:HB3   | 13       | 0.12          |
| (1,517) | 1:33:A:VAL:HB   | 1:8:A:SER:HA    | 10       | 0.12          |
| (1,510) | 1:45:A:THR:HB   | 1:46:A:SER:H    | 3        | 0.12          |
| (1,495) | 1:30:A:ILE:HG22 | 1:47:A:ARG:HD3  | 9        | 0.12          |
| (1,458) | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 1        | 0.12          |
| (1,458) | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 8        | 0.12          |
| (1,405) | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 5        | 0.12          |
| (1,405) | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 8        | 0.12          |
| (1,356) | 1:52:A:PHE:HA   | 1:45:A:THR:HG21 | 5        | 0.12          |
| (1,338) | 1:12:A:LEU:HD12 | 1:61:A:LYS:HD2  | 11       | 0.12          |
| (1,330) | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 6        | 0.12          |
| (1,281) | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 2        | 0.12          |
| (1,281) | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 4        | 0.12          |
| (1,281) | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 14       | 0.12          |
| (1,241) | 1:14:A:SER:HA   | 1:25:A:LEU:HB2  | 13       | 0.12          |
| (1,209) | 1:61:A:LYS:HB3  | 1:61:A:LYS:HA   | 10       | 0.12          |
| (1,209) | 1:61:A:LYS:HB3  | 1:61:A:LYS:HA   | 12       | 0.12          |
| (1,184) | 1:54:A:THR:HG21 | 1:54:A:THR:HG1  | 5        | 0.12          |
| (1,175) | 1:53:A:GLY:HA3  | 1:54:A:THR:HG1  | 14       | 0.12          |
| (1,87)  | 1:39:A:ASP:HB3  | 1:39:A:ASP:H    | 6        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 12       | 0.12          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 11       | 0.12          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 10       | 0.12          |
| (1,8)    | 1:23:A:LEU:HA   | 1:23:A:LEU:HD22 | 13       | 0.12          |
| (1,1156) | 1:65:A:LEU:H    | 1:64:A:TYR:HA   | 2        | 0.11          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 2        | 0.11          |
| (1,1124) | 1:59:A:TYR:H    | 1:59:A:TYR:HB3  | 8        | 0.11          |
| (1,1112) | 1:55:A:PHE:H    | 1:42:A:PHE:HB3  | 15       | 0.11          |
| (1,1045) | 1:46:A:SER:H    | 1:50:A:LYS:H    | 11       | 0.11          |
| (1,1026) | 1:37:A:CYS:H    | 1:36:A:LYS:HB2  | 1        | 0.11          |
| (1,953)  | 1:26:A:ARG:H    | 1:15:A:TYR:H    | 1        | 0.11          |
| (1,943)  | 1:25:A:LEU:H    | 1:15:A:TYR:HB2  | 12       | 0.11          |
| (1,922)  | 1:52:A:PHE:H    | 1:23:A:LEU:HD22 | 14       | 0.11          |
| (1,916)  | 1:40:A:GLY:H    | 1:42:A:PHE:HD1  | 8        | 0.11          |
| (1,916)  | 1:40:A:GLY:H    | 1:42:A:PHE:HD1  | 9        | 0.11          |
| (1,899)  | 1:31:A:VAL:H    | 1:30:A:ILE:HG13 | 8        | 0.11          |
| (1,897)  | 1:31:A:VAL:H    | 1:30:A:ILE:HB   | 3        | 0.11          |
| (1,886)  | 1:45:A:THR:H    | 1:45:A:THR:HB   | 14       | 0.11          |
| (1,837)  | 1:5:A:ASP:H     | 1:4:A:GLN:HB3   | 12       | 0.11          |
| (1,785)  | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 4        | 0.11          |
| (1,758)  | 1:20:A:ASP:H    | 1:22:A:GLU:H    | 3        | 0.11          |
| (1,629)  | 1:58:A:ASN:HB2  | 1:41:A:TRP:HE3  | 9        | 0.11          |
| (1,587)  | 1:50:A:LYS:HE2  | 1:47:A:ARG:HA   | 11       | 0.11          |
| (1,587)  | 1:50:A:LYS:HE2  | 1:47:A:ARG:HA   | 14       | 0.11          |
| (1,580)  | 1:50:A:LYS:HA   | 1:45:A:THR:HG21 | 15       | 0.11          |
| (1,560)  | 1:47:A:ARG:HD3  | 1:47:A:ARG:HA   | 2        | 0.11          |
| (1,560)  | 1:47:A:ARG:HD3  | 1:47:A:ARG:HA   | 14       | 0.11          |
| (1,557)  | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 11       | 0.11          |
| (1,557)  | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 12       | 0.11          |
| (1,538)  | 1:37:A:CYS:HB2  | 1:40:A:GLY:H    | 7        | 0.11          |
| (1,533)  | 1:36:A:LYS:HD2  | 1:42:A:PHE:HE1  | 15       | 0.11          |
| (1,518)  | 1:33:A:VAL:HB   | 1:7:A:PHE:HB3   | 4        | 0.11          |
| (1,518)  | 1:33:A:VAL:HB   | 1:7:A:PHE:HB3   | 5        | 0.11          |
| (1,518)  | 1:33:A:VAL:HB   | 1:7:A:PHE:HB3   | 7        | 0.11          |
| (1,510)  | 1:45:A:THR:HB   | 1:46:A:SER:H    | 6        | 0.11          |
| (1,510)  | 1:45:A:THR:HB   | 1:46:A:SER:H    | 15       | 0.11          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 7        | 0.11          |
| (1,496)  | 1:8:A:SER:HB2   | 1:30:A:ILE:HG22 | 14       | 0.11          |
| (1,486)  | 1:30:A:ILE:HD12 | 1:10:A:GLN:HE22 | 2        | 0.11          |
| (1,475)  | 1:26:A:ARG:HB2  | 1:26:A:ARG:HD2  | 14       | 0.11          |
| (1,458)  | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 3        | 0.11          |
| (1,458)  | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 4        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,342)  | 1:12:A:LEU:HD12 | 1:61:A:LYS:HE2  | 14       | 0.11          |
| (1,330)  | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 12       | 0.11          |
| (1,330)  | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 13       | 0.11          |
| (1,289)  | 1:10:A:GLN:HA   | 1:10:A:GLN:HG2  | 2        | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 3        | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 5        | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 6        | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 7        | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 8        | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 9        | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 10       | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 11       | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 12       | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 13       | 0.11          |
| (1,281)  | 1:9:A:TYR:HB2   | 1:9:A:TYR:HE1   | 15       | 0.11          |
| (1,244)  | 1:14:A:SER:HA   | 1:27:A:ASP:H    | 1        | 0.11          |
| (1,244)  | 1:14:A:SER:HA   | 1:27:A:ASP:H    | 2        | 0.11          |
| (1,244)  | 1:14:A:SER:HA   | 1:27:A:ASP:H    | 3        | 0.11          |
| (1,209)  | 1:61:A:LYS:HB3  | 1:61:A:LYS:HA   | 4        | 0.11          |
| (1,209)  | 1:61:A:LYS:HB3  | 1:61:A:LYS:HA   | 13       | 0.11          |
| (1,209)  | 1:61:A:LYS:HB3  | 1:61:A:LYS:HA   | 15       | 0.11          |
| (1,165)  | 1:51:A:GLN:HG2  | 1:23:A:LEU:HD22 | 5        | 0.11          |
| (1,144)  | 1:48:A:ARG:HD3  | 1:48:A:ARG:HB2  | 4        | 0.11          |
| (1,142)  | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 8        | 0.11          |
| (1,142)  | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 13       | 0.11          |
| (1,103)  | 1:42:A:PHE:HB3  | 1:33:A:VAL:HG22 | 3        | 0.11          |
| (1,66)   | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 5        | 0.11          |
| (1,56)   | 1:60:A:VAL:HG12 | 1:11:A:ALA:HB2  | 1        | 0.11          |
| (1,37)   | 1:28:A:GLY:HA3  | 1:10:A:GLN:HG2  | 10       | 0.11          |
| (1,20)   | 1:24:A:GLU:HG2  | 1:16:A:ILE:HD12 | 5        | 0.11          |
| (1,11)   | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 2        | 0.11          |
| (1,8)    | 1:23:A:LEU:HA   | 1:23:A:LEU:HD22 | 8        | 0.11          |
| (1,1154) | 1:64:A:TYR:H    | 1:63:A:LEU:HD12 | 3        | 0.1           |
| (1,1154) | 1:64:A:TYR:H    | 1:63:A:LEU:HD12 | 6        | 0.1           |
| (1,1154) | 1:64:A:TYR:H    | 1:63:A:LEU:HD12 | 15       | 0.1           |
| (1,1045) | 1:46:A:SER:H    | 1:50:A:LYS:H    | 4        | 0.1           |
| (1,1045) | 1:46:A:SER:H    | 1:50:A:LYS:H    | 10       | 0.1           |
| (1,1043) | 1:45:A:THR:H    | 1:31:A:VAL:HG12 | 6        | 0.1           |
| (1,1026) | 1:37:A:CYS:H    | 1:36:A:LYS:HB2  | 10       | 0.1           |
| (1,916)  | 1:40:A:GLY:H    | 1:42:A:PHE:HD1  | 1        | 0.1           |
| (1,916)  | 1:40:A:GLY:H    | 1:42:A:PHE:HD1  | 6        | 0.1           |
| (1,916)  | 1:40:A:GLY:H    | 1:42:A:PHE:HD1  | 15       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,890) | 1:54:A:THR:H    | 1:54:A:THR:HG21 | 14       | 0.1           |
| (1,886) | 1:45:A:THR:H    | 1:45:A:THR:HB   | 6        | 0.1           |
| (1,793) | 1:53:A:GLY:H    | 1:52:A:PHE:HD2  | 2        | 0.1           |
| (1,785) | 1:25:A:LEU:H    | 1:24:A:GLU:HG2  | 1        | 0.1           |
| (1,739) | 1:15:A:TYR:H    | 1:15:A:TYR:HD1  | 12       | 0.1           |
| (1,700) | 1:5:A:ASP:HB2   | 1:6:A:LEU:H     | 5        | 0.1           |
| (1,593) | 1:54:A:THR:HB   | 1:55:A:PHE:HA   | 5        | 0.1           |
| (1,587) | 1:50:A:LYS:HE2  | 1:47:A:ARG:HA   | 10       | 0.1           |
| (1,576) | 1:49:A:THR:HB   | 1:46:A:SER:HB2  | 9        | 0.1           |
| (1,576) | 1:49:A:THR:HB   | 1:46:A:SER:HB2  | 12       | 0.1           |
| (1,557) | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 10       | 0.1           |
| (1,557) | 1:23:A:LEU:HG   | 1:46:A:SER:HB2  | 14       | 0.1           |
| (1,458) | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 6        | 0.1           |
| (1,458) | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 10       | 0.1           |
| (1,458) | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 11       | 0.1           |
| (1,458) | 1:25:A:LEU:HB2  | 1:15:A:TYR:HB3  | 15       | 0.1           |
| (1,405) | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 11       | 0.1           |
| (1,405) | 1:18:A:GLN:HA   | 1:19:A:ASN:HB2  | 15       | 0.1           |
| (1,343) | 1:12:A:LEU:HA   | 1:12:A:LEU:HG   | 8        | 0.1           |
| (1,341) | 1:12:A:LEU:HD12 | 1:12:A:LEU:HG   | 8        | 0.1           |
| (1,330) | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 1        | 0.1           |
| (1,330) | 1:12:A:LEU:HD12 | 1:60:A:VAL:H    | 11       | 0.1           |
| (1,329) | 1:12:A:LEU:HD12 | 1:13:A:TYR:HD1  | 6        | 0.1           |
| (1,309) | 1:59:A:TYR:HA   | 1:12:A:LEU:HD12 | 8        | 0.1           |
| (1,231) | 1:63:A:LEU:HA   | 1:64:A:TYR:H    | 6        | 0.1           |
| (1,209) | 1:61:A:LYS:HB3  | 1:61:A:LYS:HA   | 3        | 0.1           |
| (1,142) | 1:47:A:ARG:HB2  | 1:47:A:ARG:HD3  | 2        | 0.1           |
| (1,87)  | 1:39:A:ASP:HB3  | 1:39:A:ASP:H    | 2        | 0.1           |
| (1,66)  | 1:34:A:MET:HG2  | 1:34:A:MET:HA   | 13       | 0.1           |
| (1,36)  | 1:27:A:ASP:HB3  | 1:13:A:TYR:HA   | 12       | 0.1           |
| (1,11)  | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 6        | 0.1           |
| (1,11)  | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 7        | 0.1           |
| (1,11)  | 1:35:A:GLU:HA   | 1:35:A:GLU:HG2  | 15       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found