



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 06:04 PM UTC

PDB ID : 2LWF / pdb\_00002lwf  
BMRB ID : 18624  
Title : Structure of N-terminal domain of a plant Grx  
Authors : Feng, Y.  
Deposited on : 2012-07-28

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
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

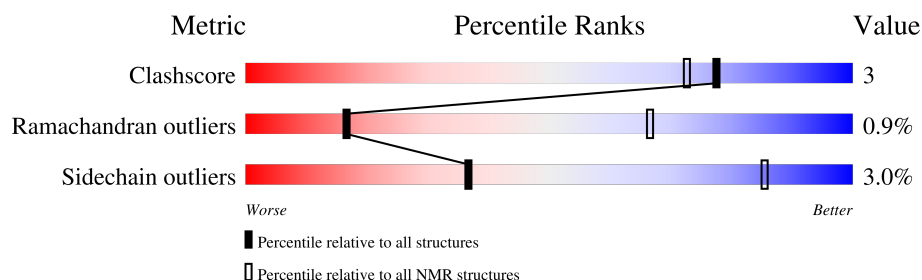
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 94%.

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     | 119    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:67-A:161 (95)       | 0.59              | 9            |

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1828 atoms, of which 919 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Monothiol glutaredoxin-S16, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 119      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1828  | 576 | 919 | 156 | 175 | 2 |       |

There are 11 discrepancies between the modelled and reference sequences:

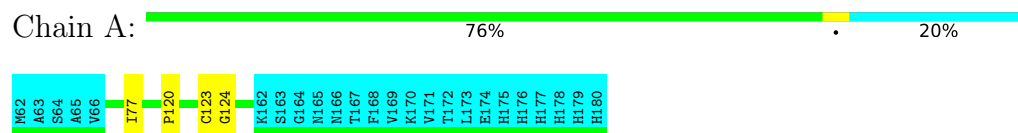
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 62      | MET      | -      | initiating methionine | UNP Q8H7F6 |
| A     | 171     | VAL      | -      | expression tag        | UNP Q8H7F6 |
| A     | 172     | THR      | -      | expression tag        | UNP Q8H7F6 |
| A     | 173     | LEU      | -      | expression tag        | UNP Q8H7F6 |
| A     | 174     | GLU      | -      | expression tag        | UNP Q8H7F6 |
| A     | 175     | HIS      | -      | expression tag        | UNP Q8H7F6 |
| A     | 176     | HIS      | -      | expression tag        | UNP Q8H7F6 |
| A     | 177     | HIS      | -      | expression tag        | UNP Q8H7F6 |
| A     | 178     | HIS      | -      | expression tag        | UNP Q8H7F6 |
| A     | 179     | HIS      | -      | expression tag        | UNP Q8H7F6 |
| A     | 180     | HIS      | -      | expression tag        | UNP Q8H7F6 |

## 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: Monothiol glutaredoxin-S16, chloroplastic

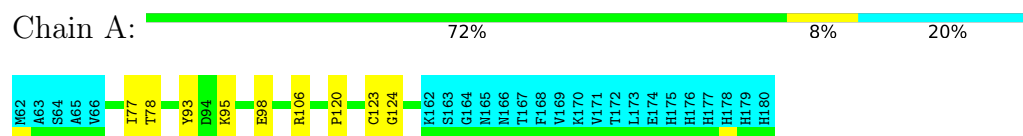


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

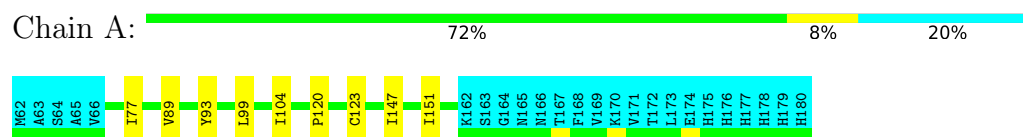
#### 4.2.1 Score per residue for model 1

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



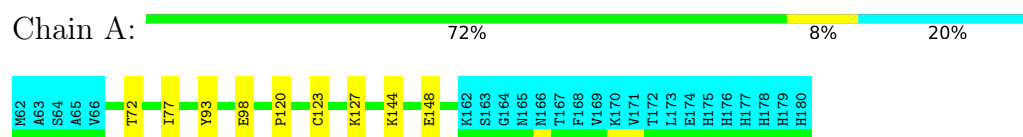
#### 4.2.2 Score per residue for model 2

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



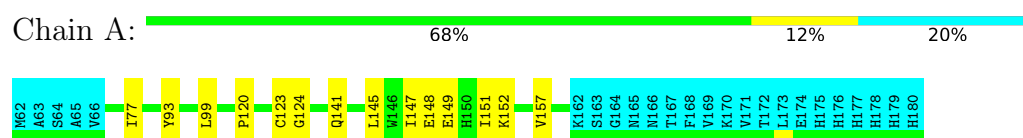
### 4.2.3 Score per residue for model 3

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



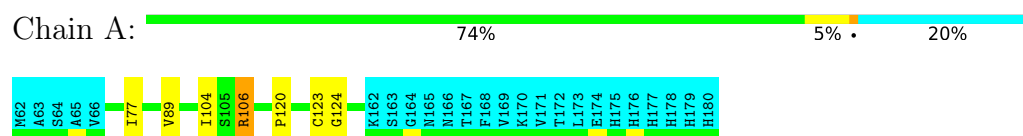
### 4.2.4 Score per residue for model 4

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



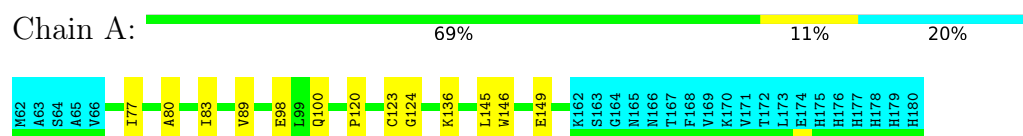
### 4.2.5 Score per residue for model 5

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



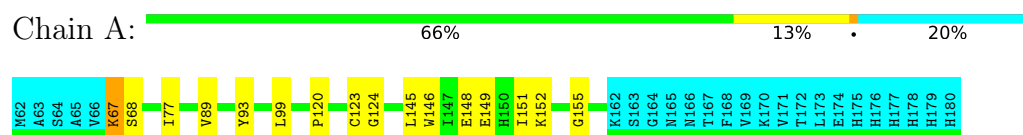
### 4.2.6 Score per residue for model 6

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



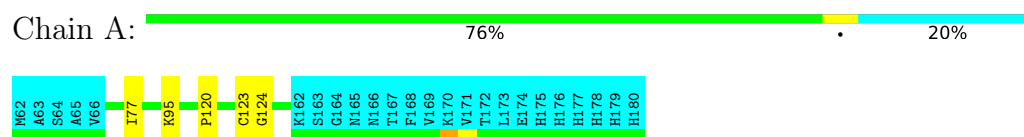
### 4.2.7 Score per residue for model 7

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



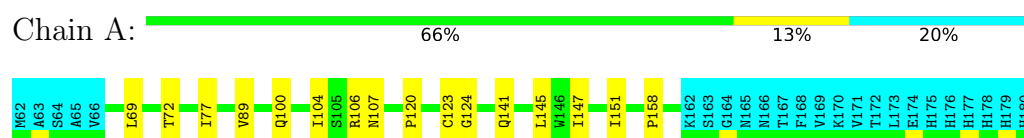
### 4.2.8 Score per residue for model 8

- Molecule 1: Monothiol glutaredoxin-S16, chloroplatic



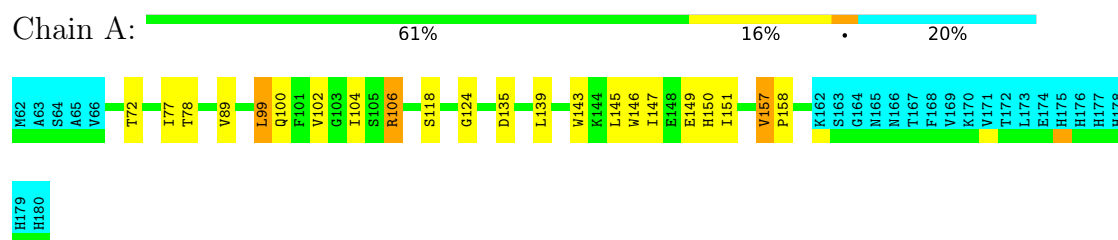
### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Monothiol glutaredoxin-S16, chloroplatic



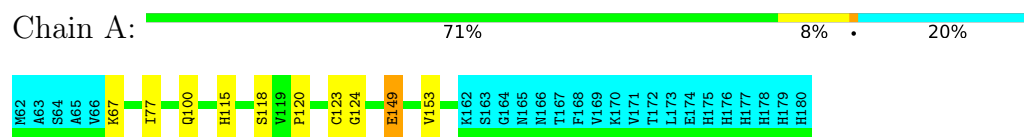
### 4.2.10 Score per residue for model 10

- Molecule 1: Monothiol glutaredoxin-S16, chloroplatic



### 4.2.11 Score per residue for model 11

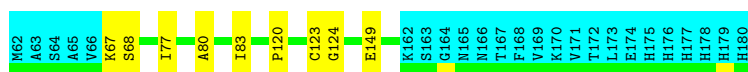
- Molecule 1: Monothiol glutaredoxin-S16, chloroplatic



### 4.2.12 Score per residue for model 12

- Molecule 1: Monothiol glutaredoxin-S16, chloroplatic





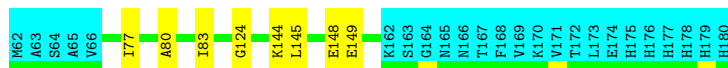
#### 4.2.13 Score per residue for model 13

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



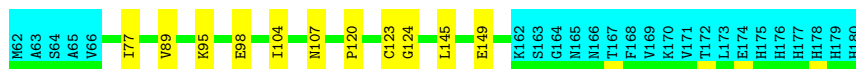
#### 4.2.14 Score per residue for model 14

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



#### 4.2.15 Score per residue for model 15

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



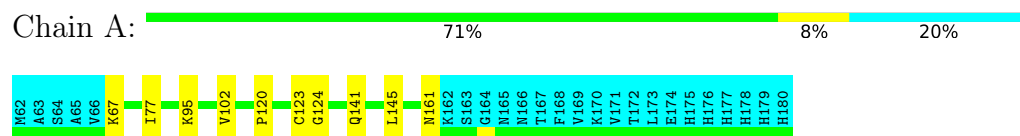
#### 4.2.16 Score per residue for model 16

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



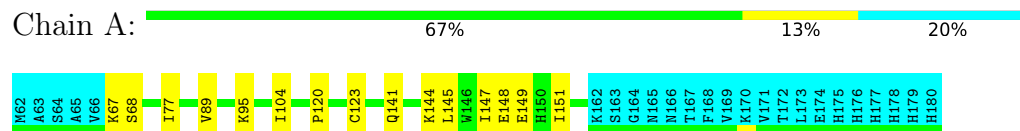
#### 4.2.17 Score per residue for model 17

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



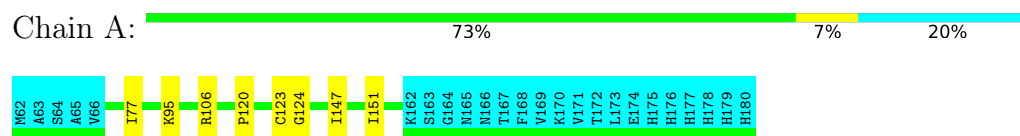
#### 4.2.18 Score per residue for model 18

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



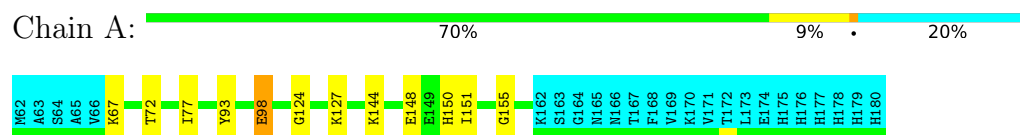
#### 4.2.19 Score per residue for model 19

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



#### 4.2.20 Score per residue for model 20

- Molecule 1: Monothiol glutaredoxin-S16, chloroplastic



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CNS           | structure solution |         |
| CNS           | refinement         |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1370           |
| Number of shifts mapped to atoms             | 1370           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 94%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.04±0.03    | 0±0/732 ( 0.0± 0.0%) | 0.98±0.03   | 0±0/999 ( 0.0± 0.0%) |
| All | All   | 1.04         | 0/14640 ( 0.0%)      | 0.98        | 3/19980 ( 0.0%)      |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.1±0.3   |
| All | All   | 0         | 2         |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 106 | ARG  | N-CA-C | -5.23 | 106.75      | 113.23   | 9      | 2     |
| 1   | A     | 67  | LYS  | N-CA-C | -5.18 | 106.91      | 113.43   | 17     | 1     |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 106 | ARG  | Sidechain | 2              |

### 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     | 717   | 732      | 730      | 4±2     |
| All | All   | 14340 | 14640    | 14600    | 84      |

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 3.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:120:PRO:HA   | 1:A:123:CYS:SG   | 0.73     | 2.23        | 12     | 17    |
| 1:A:68:SER:HB3   | 1:A:149:GLU:OE1  | 0.55     | 2.02        | 18     | 1     |
| 1:A:144:LYS:O    | 1:A:148:GLU:HG3  | 0.54     | 2.02        | 20     | 2     |
| 1:A:106:ARG:HD3  | 1:A:106:ARG:O    | 0.52     | 2.03        | 1      | 1     |
| 1:A:148:GLU:O    | 1:A:152:LYS:HG2  | 0.51     | 2.05        | 7      | 1     |
| 1:A:93:TYR:CE2   | 1:A:99:LEU:HB2   | 0.51     | 2.40        | 2      | 3     |
| 1:A:147:ILE:O    | 1:A:151:ILE:HG12 | 0.51     | 2.05        | 16     | 4     |
| 1:A:106:ARG:HD2  | 1:A:106:ARG:C    | 0.49     | 2.33        | 19     | 1     |
| 1:A:145:LEU:O    | 1:A:149:GLU:HG2  | 0.49     | 2.08        | 10     | 6     |
| 1:A:141:GLN:O    | 1:A:145:LEU:HG   | 0.48     | 2.08        | 9      | 4     |
| 1:A:72:THR:HG21  | 1:A:146:TRP:CH2  | 0.48     | 2.43        | 10     | 1     |
| 1:A:89:VAL:HB    | 1:A:146:TRP:CH2  | 0.47     | 2.44        | 13     | 1     |
| 1:A:147:ILE:O    | 1:A:151:ILE:HG13 | 0.47     | 2.09        | 10     | 4     |
| 1:A:93:TYR:HA    | 1:A:98:GLU:O     | 0.47     | 2.09        | 20     | 3     |
| 1:A:89:VAL:HG12  | 1:A:104:ILE:HG22 | 0.47     | 1.85        | 9      | 6     |
| 1:A:149:GLU:O    | 1:A:153:VAL:HG12 | 0.46     | 2.11        | 11     | 1     |
| 1:A:144:LYS:HE3  | 1:A:148:GLU:OE1  | 0.45     | 2.10        | 18     | 1     |
| 1:A:100:GLN:O    | 1:A:158:PRO:HG2  | 0.44     | 2.12        | 9      | 2     |
| 1:A:102:VAL:HG22 | 1:A:161:ASN:HD21 | 0.44     | 1.72        | 17     | 1     |
| 1:A:72:THR:CG2   | 1:A:127:LYS:HB3  | 0.43     | 2.43        | 3      | 3     |
| 1:A:151:ILE:O    | 1:A:155:GLY:HA2  | 0.43     | 2.12        | 20     | 2     |
| 1:A:80:ALA:HA    | 1:A:83:ILE:HG12  | 0.43     | 1.89        | 12     | 4     |
| 1:A:148:GLU:O    | 1:A:152:LYS:HG3  | 0.43     | 2.13        | 4      | 1     |
| 1:A:141:GLN:O    | 1:A:145:LEU:HD22 | 0.43     | 2.14        | 18     | 1     |
| 1:A:68:SER:HB2   | 1:A:149:GLU:OE2  | 0.42     | 2.15        | 12     | 1     |
| 1:A:89:VAL:HG13  | 1:A:146:TRP:CH2  | 0.42     | 2.48        | 7      | 2     |
| 1:A:95:LYS:HE3   | 1:A:123:CYS:O    | 0.41     | 2.15        | 18     | 1     |
| 1:A:99:LEU:HB3   | 1:A:150:HIS:CG   | 0.41     | 2.50        | 10     | 1     |
| 1:A:144:LYS:O    | 1:A:148:GLU:HG2  | 0.41     | 2.16        | 14     | 1     |
| 1:A:102:VAL:HG23 | 1:A:143:TRP:NE1  | 0.41     | 2.31        | 10     | 1     |
| 1:A:67:LYS:HE2   | 1:A:67:LYS:HA    | 0.41     | 1.92        | 18     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:102:VAL:HG21 | 1:A:147:ILE:HB  | 0.41     | 1.92        | 10     | 1     |
| 1:A:68:SER:HA    | 1:A:146:TRP:CD1 | 0.40     | 2.51        | 7      | 1     |
| 1:A:135:ASP:O    | 1:A:139:LEU:HG  | 0.40     | 2.15        | 10     | 1     |
| 1:A:69:LEU:HA    | 1:A:72:THR:OG1  | 0.40     | 2.17        | 9      | 1     |
| 1:A:115:HIS:HA   | 1:A:118:SER:OG  | 0.40     | 2.16        | 11     | 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     | 95/119 (80%)    | 88±2 (92±2%) | 7±2 (7±2%) | 1±0 (1±1%) | 16          | 66 |
| All | All   | 1900/2380 (80%) | 1752 (92%)   | 131 (7%)   | 17 (1%)    | 16          | 66 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 124 | GLY  | 16             |
| 1   | A     | 67  | LYS  | 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     | 81/102 (79%)    | 79±1 (97±1%) | 2±1 (3±1%) | 37          | 85 |
| All | All   | 1620/2040 (79%) | 1572 (97%)   | 48 (3%)    | 37          | 85 |

All 15 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 77  | ILE  | 20             |
| 1   | A     | 95  | LYS  | 5              |
| 1   | A     | 67  | LYS  | 4              |
| 1   | A     | 157 | VAL  | 3              |
| 1   | A     | 98  | GLU  | 3              |
| 1   | A     | 78  | THR  | 2              |
| 1   | A     | 100 | GLN  | 2              |
| 1   | A     | 107 | ASN  | 2              |
| 1   | A     | 106 | ARG  | 1              |
| 1   | A     | 136 | LYS  | 1              |
| 1   | A     | 99  | LEU  | 1              |
| 1   | A     | 149 | GLU  | 1              |
| 1   | A     | 97  | ASP  | 1              |
| 1   | A     | 154 | THR  | 1              |
| 1   | A     | 150 | HIS  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

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 94% for the well-defined parts and 87% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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                  | 1370 |
| Number of shifts mapped to atoms        | 1370 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 112      | $-0.23 \pm 0.13$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 105      | $0.07 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 102      | $-0.05 \pm 0.18$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 103      | $0.20 \pm 0.27$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1166 atoms were assigned a chemical shift out of a possible 1247. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 458/469 (98%) | 188/190 (99%) | 182/190 (96%)   | 88/89 (99%)     |
| Sidechain | 652/710 (92%) | 445/467 (95%) | 203/228 (89%)   | 4/15 (27%)      |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 56/68 (82%)     | 28/33 (85%)    | 26/29 (90%)     | 2/6 (33%)       |
| Overall  | 1166/1247 (94%) | 661/690 (96%)  | 411/447 (92%)   | 94/110 (85%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1370 atoms were assigned a chemical shift out of a possible 1573. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 538/590 (91%)   | 221/239 (92%)  | 214/238 (90%)   | 103/113 (91%)   |
| Sidechain | 766/857 (89%)   | 522/564 (93%)  | 238/274 (87%)   | 6/19 (32%)      |
| Aromatic  | 66/126 (52%)    | 33/62 (53%)    | 31/46 (67%)     | 2/18 (11%)      |
| Overall   | 1370/1573 (87%) | 776/865 (90%)  | 483/558 (87%)   | 111/150 (74%)   |

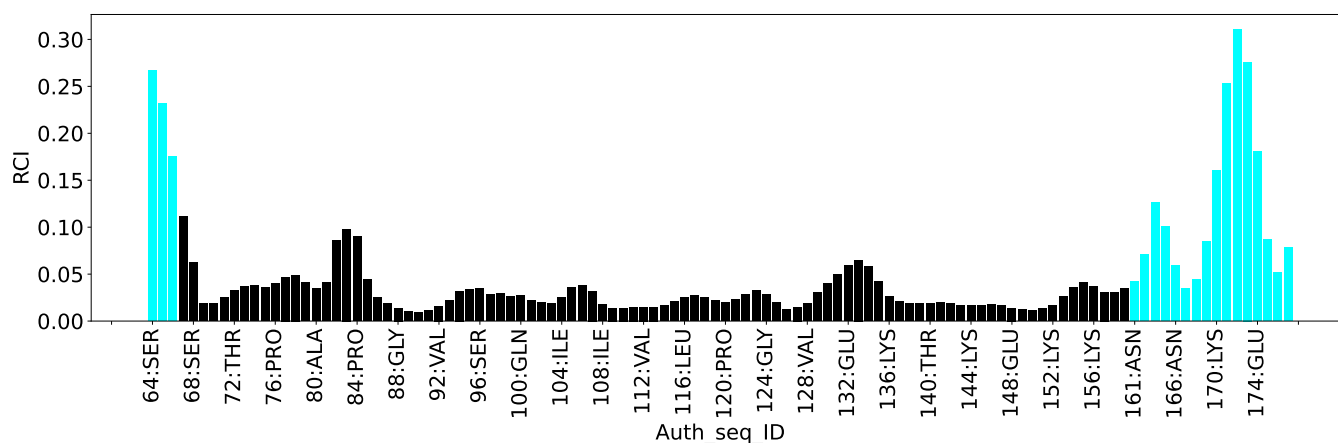
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 2999  |
| Intra-residue ( $ i-j =0$ )                              | 892   |
| Sequential ( $ i-j =1$ )                                 | 752   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 498   |
| Long range ( $ i-j \geq 5$ )                             | 783   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 74    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 170   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 26.6  |
| Number of long range restraints per residue <sup>1</sup> | 6.8   |

<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)  | 30.6                                   | 0.2     |
| 0.2-0.5 (Medium) | 65.5                                   | 0.5     |
| >0.5 (Large)     | 63.8                                   | 4.37    |

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

Dihedral-angle violations less than 1° are not included in the calculation.

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 2.0                                    | 3.29    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

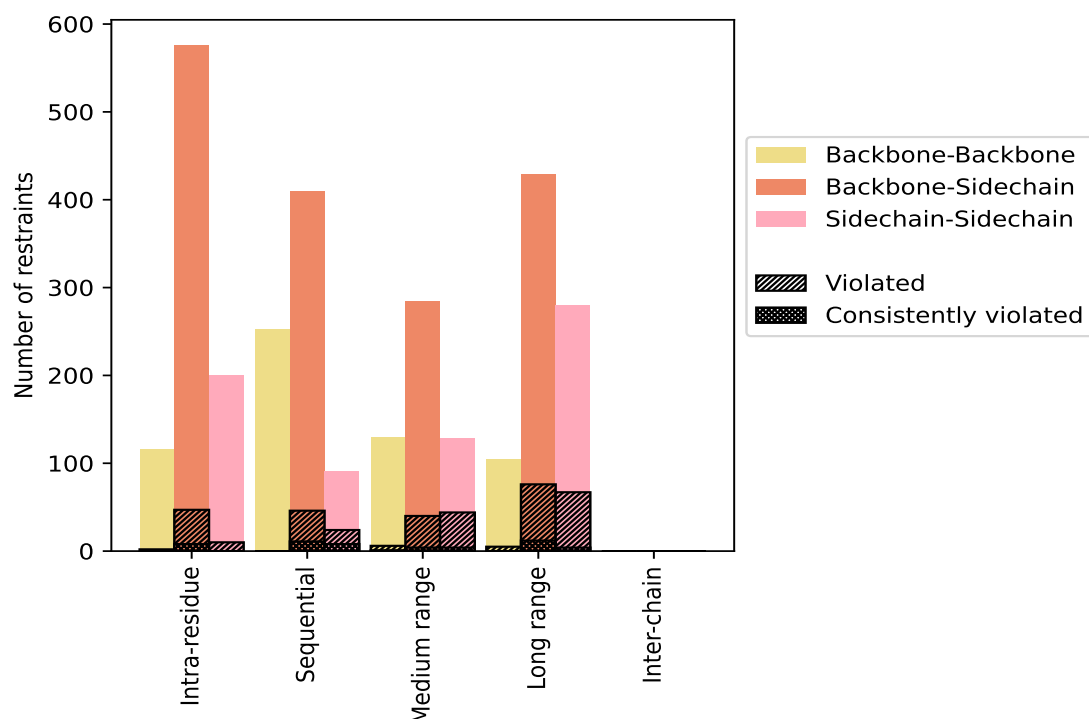
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>892</b>  | <b>29.7</b>    | <b>59</b>             | <b>6.6</b>     | <b>2.0</b>     | <b>8</b>                           | <b>0.9</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 116         | 3.9            | 2                     | 1.7            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 576         | 19.2           | 47                    | 8.2            | 1.6            | 8                                  | 1.4            | 0.3            |
| Sidechain-Sidechain                                                         | 200         | 6.7            | 10                    | 5.0            | 0.3            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>752</b>  | <b>25.1</b>    | <b>70</b>             | <b>9.3</b>     | <b>2.3</b>     | <b>19</b>                          | <b>2.5</b>     | <b>0.6</b>     |
| Backbone-Backbone                                                           | 252         | 8.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 409         | 13.6           | 46                    | 11.2           | 1.5            | 11                                 | 2.7            | 0.4            |
| Sidechain-Sidechain                                                         | 91          | 3.0            | 24                    | 26.4           | 0.8            | 8                                  | 8.8            | 0.3            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>498</b>  | <b>16.6</b>    | <b>90</b>             | <b>18.1</b>    | <b>3.0</b>     | <b>9</b>                           | <b>1.8</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 130         | 4.3            | 6                     | 4.6            | 0.2            | 1                                  | 0.8            | 0.0            |
| Backbone-Sidechain                                                          | 240         | 8.0            | 40                    | 16.7           | 1.3            | 4                                  | 1.7            | 0.1            |
| Sidechain-Sidechain                                                         | 128         | 4.3            | 44                    | 34.4           | 1.5            | 4                                  | 3.1            | 0.1            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>783</b>  | <b>26.1</b>    | <b>148</b>            | <b>18.9</b>    | <b>4.9</b>     | <b>16</b>                          | <b>2.0</b>     | <b>0.5</b>     |
| Backbone-Backbone                                                           | 104         | 3.5            | 5                     | 4.8            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 399         | 13.3           | 76                    | 19.0           | 2.5            | 12                                 | 3.0            | 0.4            |
| Sidechain-Sidechain                                                         | 280         | 9.3            | 67                    | 23.9           | 2.2            | 4                                  | 1.4            | 0.1            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>74</b>   | <b>2.5</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>2999</b> | <b>100.0</b>   | <b>367</b>            | <b>12.2</b>    | <b>12.2</b>    | <b>52</b>                          | <b>1.7</b>     | <b>1.7</b>     |
| Backbone-Backbone                                                           | 602         | 20.1           | 13                    | 2.2            | 0.4            | 1                                  | 0.2            | 0.0            |
| Backbone-Sidechain                                                          | 1698        | 56.6           | 209                   | 12.3           | 7.0            | 35                                 | 2.1            | 1.2            |
| Sidechain-Sidechain                                                         | 699         | 23.3           | 145                   | 20.7           | 4.8            | 16                                 | 2.3            | 0.5            |

<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        | 25                   | 32              | 26              | 76              | 0               | 159   | 0.56     | 4.1     | 0.57                | 0.41       |
| 2        | 22                   | 30              | 30              | 73              | 0               | 155   | 0.57     | 4.3     | 0.58                | 0.42       |
| 3        | 22                   | 36              | 35              | 69              | 0               | 162   | 0.56     | 4.14    | 0.58                | 0.39       |
| 4        | 23                   | 44              | 29              | 67              | 0               | 163   | 0.59     | 3.9     | 0.57                | 0.43       |
| 5        | 22                   | 39              | 39              | 64              | 0               | 164   | 0.55     | 4.37    | 0.59                | 0.4        |
| 6        | 25                   | 37              | 31              | 53              | 0               | 146   | 0.64     | 4.22    | 0.65                | 0.46       |
| 7        | 20                   | 38              | 36              | 66              | 0               | 160   | 0.56     | 4.15    | 0.57                | 0.42       |
| 8        | 21                   | 40              | 35              | 67              | 0               | 163   | 0.56     | 4.22    | 0.58                | 0.4        |
| 9        | 25                   | 35              | 31              | 69              | 0               | 160   | 0.58     | 4.34    | 0.58                | 0.43       |
| 10       | 18                   | 35              | 32              | 66              | 0               | 151   | 0.58     | 4.34    | 0.59                | 0.42       |

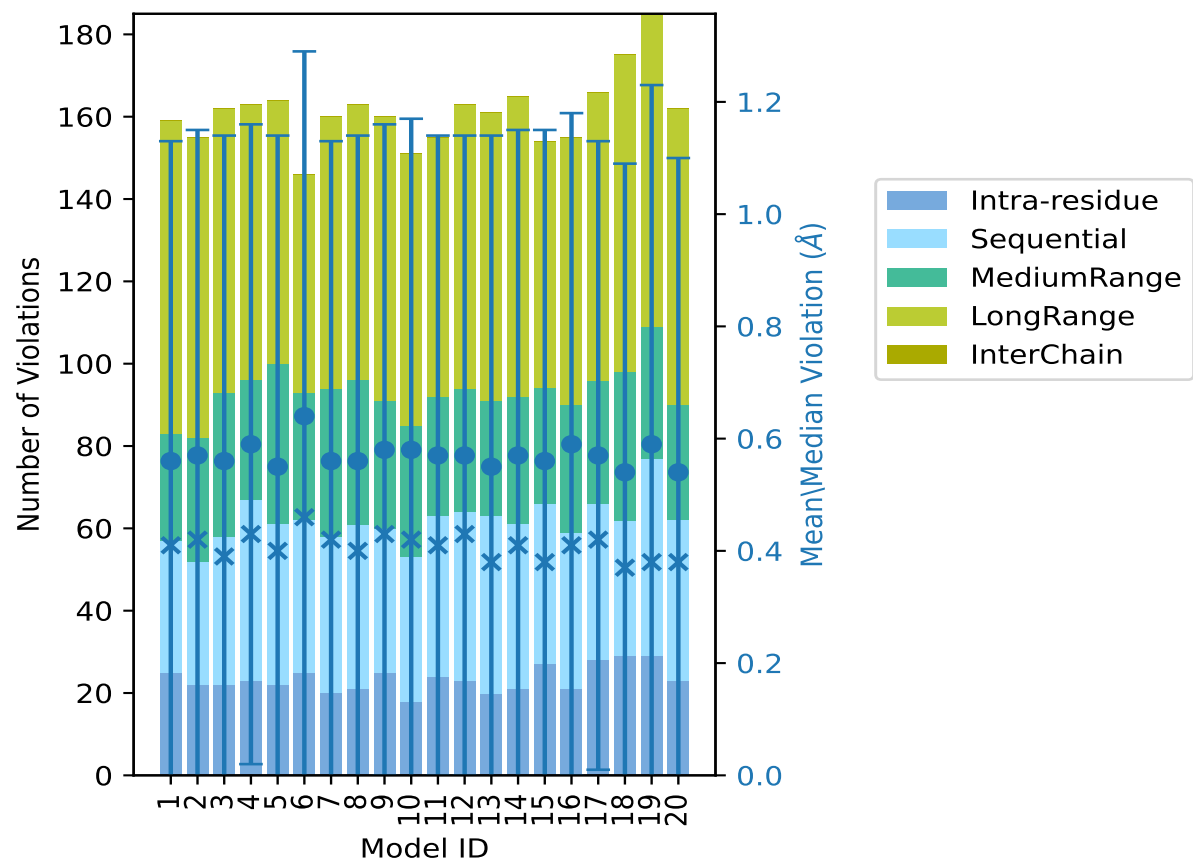
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 24                   | 39              | 29              | 63              | 0               | 155   | 0.57     | 4.28    | 0.57                | 0.41       |
| 12       | 23                   | 41              | 30              | 69              | 0               | 163   | 0.57     | 4.15    | 0.57                | 0.43       |
| 13       | 20                   | 43              | 28              | 70              | 0               | 161   | 0.55     | 4.27    | 0.59                | 0.38       |
| 14       | 21                   | 40              | 31              | 73              | 0               | 165   | 0.57     | 4.24    | 0.58                | 0.41       |
| 15       | 27                   | 39              | 28              | 60              | 0               | 154   | 0.56     | 4.34    | 0.59                | 0.38       |
| 16       | 21                   | 38              | 31              | 65              | 0               | 155   | 0.59     | 4.23    | 0.59                | 0.41       |
| 17       | 28                   | 38              | 30              | 70              | 0               | 166   | 0.57     | 4.34    | 0.56                | 0.42       |
| 18       | 29                   | 33              | 36              | 77              | 0               | 175   | 0.54     | 4.3     | 0.55                | 0.37       |
| 19       | 29                   | 48              | 32              | 76              | 0               | 185   | 0.59     | 4.15    | 0.64                | 0.38       |
| 20       | 23                   | 39              | 28              | 72              | 0               | 162   | 0.54     | 4.26    | 0.56                | 0.38       |

<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

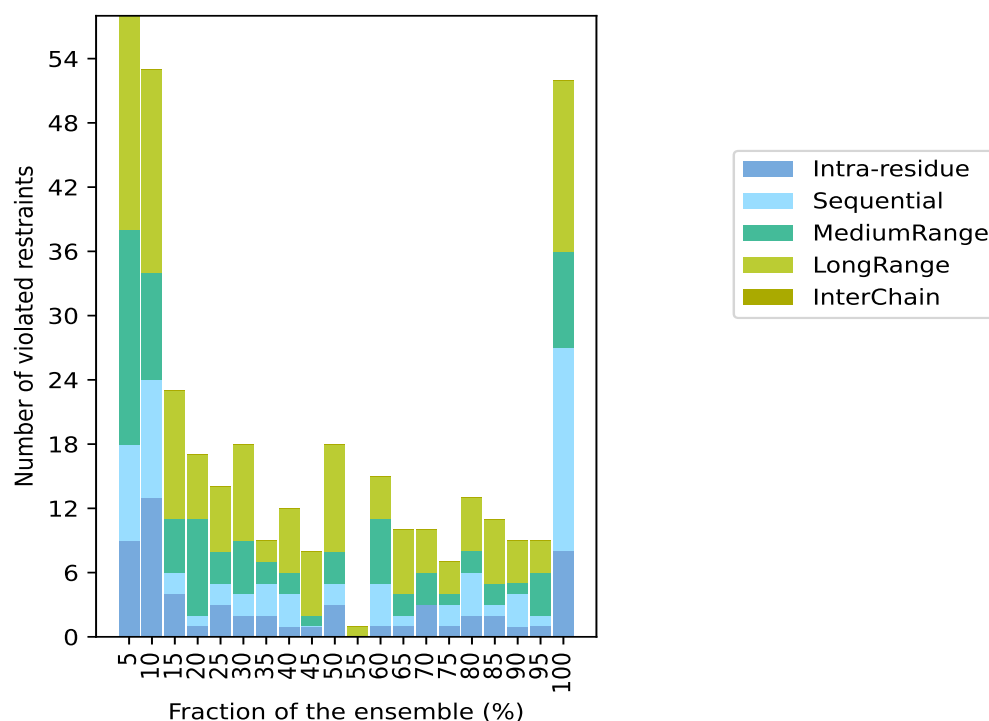
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2558(IR:833, SQ:682, MR:408, LR:635, IC:0) restraints are 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>       | %     |
| 9                             | 9               | 20              | 20              | 0               | 58    | 1                        | 5.0   |
| 13                            | 11              | 10              | 19              | 0               | 53    | 2                        | 10.0  |
| 4                             | 2               | 5               | 12              | 0               | 23    | 3                        | 15.0  |
| 1                             | 1               | 9               | 6               | 0               | 17    | 4                        | 20.0  |
| 3                             | 2               | 3               | 6               | 0               | 14    | 5                        | 25.0  |
| 2                             | 2               | 5               | 9               | 0               | 18    | 6                        | 30.0  |
| 2                             | 3               | 2               | 2               | 0               | 9     | 7                        | 35.0  |
| 1                             | 3               | 2               | 6               | 0               | 12    | 8                        | 40.0  |
| 1                             | 0               | 1               | 6               | 0               | 8     | 9                        | 45.0  |
| 3                             | 2               | 3               | 10              | 0               | 18    | 10                       | 50.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 11                       | 55.0  |
| 1                             | 4               | 6               | 4               | 0               | 15    | 12                       | 60.0  |
| 1                             | 1               | 2               | 6               | 0               | 10    | 13                       | 65.0  |
| 3                             | 0               | 3               | 4               | 0               | 10    | 14                       | 70.0  |
| 1                             | 2               | 1               | 3               | 0               | 7     | 15                       | 75.0  |
| 2                             | 4               | 2               | 5               | 0               | 13    | 16                       | 80.0  |
| 2                             | 1               | 2               | 6               | 0               | 11    | 17                       | 85.0  |
| 1                             | 3               | 1               | 4               | 0               | 9     | 18                       | 90.0  |
| 1                             | 1               | 4               | 3               | 0               | 9     | 19                       | 95.0  |
| 8                             | 19              | 9               | 16              | 0               | 52    | 20                       | 100.0 |

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

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

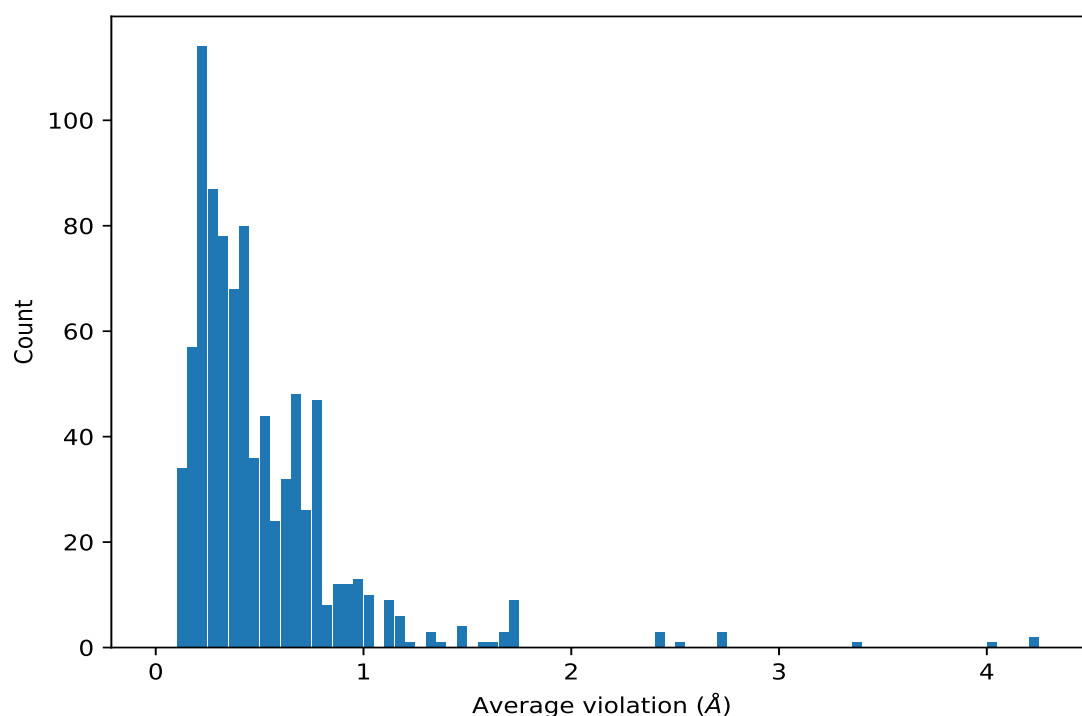
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1           | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|----------------|---------------------|----------|---------------------|------------|
| (1,232)  | 1:105:A:SER:H    | 1:90:A:TYR:HD1 | 20                  | 4.22     | 0.13                | 4.25       |
| (1,232)  | 1:105:A:SER:H    | 1:90:A:TYR:HE1 | 20                  | 4.22     | 0.13                | 4.25       |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1 | 20                  | 4.01     | 0.09                | 4.0        |
| (1,1769) | 1:104:A:ILE:HG21 | 1:90:A:TYR:HD1 | 20                  | 2.72     | 0.15                | 2.74       |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1 | 20                  | 2.72     | 0.15                | 2.74       |
| (1,1769) | 1:104:A:ILE:HG23 | 1:90:A:TYR:HD1 | 20                  | 2.72     | 0.15                | 2.74       |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 20                  | 2.42     | 0.12                | 2.42       |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 20                  | 2.42     | 0.12                | 2.42       |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 20                  | 2.42     | 0.12                | 2.42       |
| (1,1419) | 1:92:A:VAL:HG12  | 1:101:A:PHE:H  | 20                  | 1.74     | 0.2                 | 1.74       |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H  | 20                  | 1.74     | 0.2                 | 1.74       |
| (1,1419) | 1:92:A:VAL:HG13  | 1:101:A:PHE:H  | 20                  | 1.74     | 0.2                 | 1.74       |
| (1,1419) | 1:92:A:VAL:HG23  | 1:101:A:PHE:H  | 20                  | 1.74     | 0.2                 | 1.74       |
| (1,1419) | 1:92:A:VAL:HG21  | 1:101:A:PHE:H  | 20                  | 1.74     | 0.2                 | 1.74       |
| (1,1419) | 1:92:A:VAL:HG22  | 1:101:A:PHE:H  | 20                  | 1.74     | 0.2                 | 1.74       |
| (1,1438) | 1:104:A:ILE:HD11 | 1:90:A:TYR:HE2 | 20                  | 1.73     | 0.2                 | 1.76       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1438) | 1:104:A:ILE:HD12 | 1:90:A:TYR:HE2   | 20                  | 1.73     | 0.2                 | 1.76       |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2   | 20                  | 1.73     | 0.2                 | 1.76       |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 20                  | 1.38     | 0.12                | 1.42       |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 20                  | 1.33     | 0.04                | 1.35       |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 20                  | 1.33     | 0.04                | 1.35       |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG13 | 20                  | 1.33     | 0.04                | 1.35       |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG23 | 20                  | 1.14     | 0.23                | 1.18       |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD11 | 20                  | 1.14     | 0.23                | 1.18       |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD13 | 20                  | 1.14     | 0.23                | 1.18       |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD21 | 20                  | 1.14     | 0.23                | 1.18       |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG21 | 20                  | 1.14     | 0.23                | 1.18       |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG22 | 20                  | 1.14     | 0.23                | 1.18       |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD22 | 20                  | 1.14     | 0.23                | 1.18       |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 20                  | 1.12     | 0.19                | 1.14       |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE2   | 20                  | 1.12     | 0.19                | 1.14       |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 20                  | 1.04     | 0.15                | 1.08       |
| (1,1830) | 1:72:A:THR:HA    | 1:70:A:THR:HG22  | 20                  | 1.04     | 0.15                | 1.08       |
| (1,1830) | 1:72:A:THR:HA    | 1:70:A:THR:HG23  | 20                  | 1.04     | 0.15                | 1.08       |
| (1,1722) | 1:69:A:LEU:HD22  | 1:150:A:HIS:HE1  | 20                  | 1.03     | 0.25                | 1.1        |
| (1,1722) | 1:69:A:LEU:HD21  | 1:149:A:GLU:H    | 20                  | 1.03     | 0.25                | 1.1        |
| (1,1722) | 1:69:A:LEU:HD22  | 1:149:A:GLU:H    | 20                  | 1.03     | 0.25                | 1.1        |
| (1,1722) | 1:69:A:LEU:HD21  | 1:150:A:HIS:HE1  | 20                  | 1.03     | 0.25                | 1.1        |
| (1,1722) | 1:69:A:LEU:HD23  | 1:149:A:GLU:H    | 20                  | 1.03     | 0.25                | 1.1        |
| (1,1722) | 1:69:A:LEU:HD23  | 1:150:A:HIS:HE1  | 20                  | 1.03     | 0.25                | 1.1        |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 20                  | 1.01     | 0.2                 | 0.96       |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG21  | 20                  | 0.99     | 0.25                | 1.02       |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD12 | 20                  | 0.99     | 0.25                | 1.02       |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG22  | 20                  | 0.99     | 0.25                | 1.02       |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD11 | 20                  | 0.99     | 0.25                | 1.02       |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD13 | 20                  | 0.99     | 0.25                | 1.02       |
| (1,92)   | 1:95:A:LYS:H     | 1:116:A:LEU:HD22 | 20                  | 0.99     | 0.25                | 1.02       |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG23  | 20                  | 0.99     | 0.25                | 1.02       |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 20                  | 0.96     | 0.17                | 0.99       |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE2   | 20                  | 0.96     | 0.17                | 0.99       |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG22  | 20                  | 0.87     | 0.24                | 0.9        |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG13  | 20                  | 0.87     | 0.24                | 0.9        |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG23  | 20                  | 0.87     | 0.24                | 0.9        |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG21  | 20                  | 0.87     | 0.24                | 0.9        |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG23 | 20                  | 0.85     | 0.1                 | 0.88       |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG22 | 20                  | 0.85     | 0.1                 | 0.88       |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 20                  | 0.85     | 0.1                 | 0.88       |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG22  | 20                  | 0.84     | 0.22                | 0.86       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 20                  | 0.84     | 0.22                | 0.86       |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG23  | 20                  | 0.84     | 0.22                | 0.86       |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 20                  | 0.75     | 0.1                 | 0.75       |
| (1,1629) | 1:77:A:ILE:HG21  | 1:120:A:PRO:HA   | 20                  | 0.75     | 0.1                 | 0.75       |
| (1,1629) | 1:77:A:ILE:HG23  | 1:78:A:THR:HA    | 20                  | 0.75     | 0.1                 | 0.75       |
| (1,1629) | 1:77:A:ILE:HG21  | 1:78:A:THR:HA    | 20                  | 0.75     | 0.1                 | 0.75       |
| (1,1629) | 1:77:A:ILE:HG22  | 1:120:A:PRO:HA   | 20                  | 0.75     | 0.1                 | 0.75       |
| (1,1629) | 1:77:A:ILE:HG23  | 1:120:A:PRO:HA   | 20                  | 0.75     | 0.1                 | 0.75       |
| (1,1592) | 1:141:A:GLN:HG3  | 1:140:A:THR:HG23 | 20                  | 0.75     | 0.11                | 0.77       |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 20                  | 0.75     | 0.11                | 0.77       |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB1  | 20                  | 0.75     | 0.11                | 0.77       |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB2  | 20                  | 0.75     | 0.11                | 0.77       |
| (1,1592) | 1:141:A:GLN:HG3  | 1:140:A:THR:HG22 | 20                  | 0.75     | 0.11                | 0.77       |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 20                  | 0.71     | 0.03                | 0.71       |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG21 | 20                  | 0.71     | 0.03                | 0.71       |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG23 | 20                  | 0.71     | 0.03                | 0.71       |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG11 | 20                  | 0.71     | 0.04                | 0.72       |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG13 | 20                  | 0.71     | 0.04                | 0.72       |
| (1,18)   | 1:112:A:VAL:H    | 1:83:A:ILE:HG23  | 20                  | 0.71     | 0.04                | 0.72       |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG12 | 20                  | 0.71     | 0.04                | 0.72       |
| (1,18)   | 1:112:A:VAL:H    | 1:83:A:ILE:HG22  | 20                  | 0.71     | 0.04                | 0.72       |
| (1,18)   | 1:112:A:VAL:H    | 1:83:A:ILE:HG21  | 20                  | 0.71     | 0.04                | 0.72       |
| (1,1824) | 1:147:A:ILE:HD11 | 1:147:A:ILE:HA   | 20                  | 0.69     | 0.04                | 0.69       |
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 20                  | 0.69     | 0.04                | 0.69       |
| (1,1824) | 1:147:A:ILE:HD13 | 1:147:A:ILE:HA   | 20                  | 0.69     | 0.04                | 0.69       |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD23  | 20                  | 0.69     | 0.26                | 0.76       |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD22  | 20                  | 0.69     | 0.26                | 0.76       |
| (1,1502) | 1:84:A:PRO:HG2   | 1:83:A:ILE:HG23  | 20                  | 0.69     | 0.26                | 0.76       |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD21  | 20                  | 0.69     | 0.26                | 0.76       |
| (1,1502) | 1:84:A:PRO:HG2   | 1:83:A:ILE:HG22  | 20                  | 0.69     | 0.26                | 0.76       |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 20                  | 0.67     | 0.04                | 0.67       |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD13  | 20                  | 0.67     | 0.04                | 0.67       |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD11  | 20                  | 0.67     | 0.04                | 0.67       |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 20                  | 0.66     | 0.12                | 0.68       |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 20                  | 0.66     | 0.05                | 0.68       |
| (1,43)   | 1:146:A:TRP:H    | 1:149:A:GLU:HG2  | 20                  | 0.66     | 0.05                | 0.68       |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG2  | 20                  | 0.66     | 0.05                | 0.68       |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD23  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD22  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG23  | 1:74:A:LEU:HD21  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG23  | 1:69:A:LEU:HD11  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG21  | 1:69:A:LEU:HD13  | 20                  | 0.62     | 0.2                 | 0.63       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1550) | 1:72:A:THR:HG23  | 1:74:A:LEU:HD22  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG22  | 1:74:A:LEU:HD22  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG23  | 1:74:A:LEU:HD23  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD21  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG22  | 1:69:A:LEU:HD11  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG22  | 1:69:A:LEU:HD13  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG23  | 1:69:A:LEU:HD12  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,1550) | 1:72:A:THR:HG21  | 1:69:A:LEU:HD11  | 20                  | 0.62     | 0.2                 | 0.63       |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 20                  | 0.61     | 0.18                | 0.64       |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG21 | 20                  | 0.61     | 0.18                | 0.64       |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG23 | 20                  | 0.61     | 0.18                | 0.64       |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 20                  | 0.58     | 0.09                | 0.6        |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 20                  | 0.58     | 0.09                | 0.6        |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG23 | 20                  | 0.58     | 0.09                | 0.6        |
| (1,1485) | 1:85:A:SER:HB3   | 1:84:A:PRO:HB2   | 20                  | 0.55     | 0.1                 | 0.56       |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 20                  | 0.55     | 0.1                 | 0.56       |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 20                  | 0.54     | 0.07                | 0.55       |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 20                  | 0.53     | 0.09                | 0.54       |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 20                  | 0.53     | 0.09                | 0.54       |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 20                  | 0.53     | 0.09                | 0.54       |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG11 | 20                  | 0.52     | 0.13                | 0.55       |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG12 | 20                  | 0.52     | 0.13                | 0.55       |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG13 | 20                  | 0.52     | 0.13                | 0.55       |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 20                  | 0.52     | 0.13                | 0.55       |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 20                  | 0.52     | 0.13                | 0.55       |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 20                  | 0.52     | 0.13                | 0.55       |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 20                  | 0.5      | 0.17                | 0.44       |
| (1,1878) | 1:147:A:ILE:HG22 | 1:148:A:GLU:HB2  | 20                  | 0.5      | 0.17                | 0.44       |
| (1,1878) | 1:147:A:ILE:HG23 | 1:148:A:GLU:HB2  | 20                  | 0.5      | 0.17                | 0.44       |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 20                  | 0.49     | 0.1                 | 0.52       |
| (1,73)   | 1:125:A:SER:H    | 1:95:A:LYS:HG3   | 20                  | 0.49     | 0.1                 | 0.52       |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 20                  | 0.49     | 0.14                | 0.49       |
| (1,2014) | 1:77:A:ILE:HD13  | 1:76:A:PRO:HG2   | 20                  | 0.49     | 0.14                | 0.49       |
| (1,2014) | 1:77:A:ILE:HD11  | 1:126:A:VAL:HB   | 20                  | 0.49     | 0.14                | 0.49       |
| (1,2014) | 1:77:A:ILE:HD12  | 1:126:A:VAL:HB   | 20                  | 0.49     | 0.14                | 0.49       |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 20                  | 0.49     | 0.04                | 0.5        |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD13  | 20                  | 0.49     | 0.04                | 0.5        |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD11  | 20                  | 0.49     | 0.04                | 0.5        |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 20                  | 0.43     | 0.06                | 0.44       |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 20                  | 0.43     | 0.06                | 0.44       |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 20                  | 0.43     | 0.06                | 0.44       |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 20                  | 0.43     | 0.03                | 0.44       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 20                  | 0.43     | 0.03                | 0.44       |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 20                  | 0.43     | 0.03                | 0.44       |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 20                  | 0.43     | 0.12                | 0.42       |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 20                  | 0.43     | 0.12                | 0.42       |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 20                  | 0.43     | 0.12                | 0.42       |
| (1,1409) | 1:73:A:GLU:HG2   | 1:74:A:LEU:HD21  | 20                  | 0.43     | 0.12                | 0.42       |
| (1,1409) | 1:73:A:GLU:HG2   | 1:74:A:LEU:HD22  | 20                  | 0.43     | 0.12                | 0.42       |
| (1,1409) | 1:73:A:GLU:HG2   | 1:74:A:LEU:HD23  | 20                  | 0.43     | 0.12                | 0.42       |
| (1,5)    | 1:107:A:ASN:H    | 1:90:A:TYR:HE2   | 20                  | 0.42     | 0.12                | 0.38       |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 20                  | 0.42     | 0.12                | 0.38       |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG21 | 20                  | 0.41     | 0.14                | 0.4        |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG22 | 20                  | 0.41     | 0.14                | 0.4        |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 20                  | 0.41     | 0.14                | 0.4        |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG21  | 20                  | 0.41     | 0.11                | 0.44       |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 20                  | 0.41     | 0.11                | 0.44       |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG22  | 20                  | 0.41     | 0.11                | 0.44       |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 20                  | 0.39     | 0.06                | 0.4        |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG3  | 20                  | 0.39     | 0.06                | 0.4        |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 20                  | 0.38     | 0.08                | 0.42       |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD12  | 20                  | 0.38     | 0.08                | 0.42       |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD13  | 20                  | 0.38     | 0.08                | 0.42       |
| (1,210)  | 1:116:A:LEU:H    | 1:112:A:VAL:HA   | 20                  | 0.36     | 0.06                | 0.37       |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 20                  | 0.36     | 0.06                | 0.37       |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 20                  | 0.35     | 0.09                | 0.35       |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG22 | 20                  | 0.35     | 0.09                | 0.35       |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG23 | 20                  | 0.35     | 0.09                | 0.35       |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 20                  | 0.34     | 0.07                | 0.34       |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG21 | 20                  | 0.34     | 0.07                | 0.34       |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG22 | 20                  | 0.34     | 0.07                | 0.34       |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 20                  | 0.34     | 0.07                | 0.34       |
| (1,1665) | 1:140:A:THR:HG21 | 1:141:A:GLN:H    | 20                  | 0.34     | 0.07                | 0.34       |
| (1,1665) | 1:140:A:THR:HG22 | 1:141:A:GLN:H    | 20                  | 0.34     | 0.07                | 0.34       |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 20                  | 0.34     | 0.08                | 0.34       |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 20                  | 0.34     | 0.08                | 0.34       |
| (1,1399) | 1:138:A:VAL:HG23 | 1:137:A:ALA:H    | 20                  | 0.34     | 0.08                | 0.34       |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 20                  | 0.15     | 0.03                | 0.15       |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 20                  | 0.15     | 0.03                | 0.15       |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 20                  | 0.15     | 0.03                | 0.15       |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG21 | 20                  | 0.15     | 0.03                | 0.15       |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG22 | 20                  | 0.15     | 0.03                | 0.15       |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG23 | 20                  | 0.15     | 0.03                | 0.15       |
| (1,1679) | 1:74:A:LEU:HD21  | 1:76:A:PRO:HG3   | 19                  | 0.9      | 0.26                | 0.93       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 19                  | 0.9      | 0.26                | 0.93       |
| (1,1679) | 1:74:A:LEU:HD22  | 1:76:A:PRO:HG3   | 19                  | 0.9      | 0.26                | 0.93       |
| (1,2012) | 1:151:A:ILE:HG21 | 1:151:A:ILE:H    | 19                  | 0.75     | 0.07                | 0.78       |
| (1,2012) | 1:151:A:ILE:HG22 | 1:151:A:ILE:H    | 19                  | 0.75     | 0.07                | 0.78       |
| (1,2012) | 1:151:A:ILE:HG22 | 1:155:A:GLY:H    | 19                  | 0.75     | 0.07                | 0.78       |
| (1,2012) | 1:151:A:ILE:HG23 | 1:151:A:ILE:H    | 19                  | 0.75     | 0.07                | 0.78       |
| (1,2012) | 1:151:A:ILE:HG21 | 1:155:A:GLY:H    | 19                  | 0.75     | 0.07                | 0.78       |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG11 | 19                  | 0.72     | 0.28                | 0.73       |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG13 | 19                  | 0.72     | 0.28                | 0.73       |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG12 | 19                  | 0.72     | 0.28                | 0.73       |
| (1,1471) | 1:117:A:LYS:HG2  | 1:116:A:LEU:HD23 | 19                  | 0.72     | 0.28                | 0.73       |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 19                  | 0.65     | 0.25                | 0.71       |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 19                  | 0.43     | 0.09                | 0.43       |
| (1,1840) | 1:86:A:ALA:HB2   | 1:88:A:GLY:H     | 19                  | 0.43     | 0.09                | 0.43       |
| (1,1840) | 1:86:A:ALA:HB1   | 1:88:A:GLY:H     | 19                  | 0.43     | 0.09                | 0.43       |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 19                  | 0.42     | 0.14                | 0.43       |
| (1,2789) | 1:90:A:TYR:HD1   | 1:102:A:VAL:HB   | 19                  | 0.42     | 0.14                | 0.43       |
| (1,2789) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HB   | 19                  | 0.42     | 0.14                | 0.43       |
| (1,1688) | 1:116:A:LEU:HD21 | 1:93:A:TYR:H     | 19                  | 0.32     | 0.14                | 0.32       |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 19                  | 0.32     | 0.14                | 0.32       |
| (1,1688) | 1:116:A:LEU:HD22 | 1:93:A:TYR:H     | 19                  | 0.32     | 0.14                | 0.32       |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 19                  | 0.26     | 0.08                | 0.27       |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD12  | 19                  | 0.26     | 0.08                | 0.27       |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD13  | 19                  | 0.26     | 0.08                | 0.27       |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 19                  | 0.26     | 0.06                | 0.26       |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG23  | 19                  | 0.26     | 0.06                | 0.26       |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG21  | 19                  | 0.26     | 0.06                | 0.26       |
| (1,1579) | 1:76:A:PRO:HB2   | 1:75:A:LEU:HD12  | 19                  | 0.26     | 0.06                | 0.26       |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 18                  | 0.76     | 0.28                | 0.74       |
| (1,1528) | 1:148:A:GLU:HG2  | 1:157:A:VAL:HG21 | 18                  | 0.76     | 0.28                | 0.74       |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG21 | 18                  | 0.67     | 0.25                | 0.68       |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HD13 | 18                  | 0.67     | 0.25                | 0.68       |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG23 | 18                  | 0.67     | 0.25                | 0.68       |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG22 | 18                  | 0.67     | 0.25                | 0.68       |
| (1,1497) | 1:130:A:ILE:HG22 | 1:131:A:VAL:H    | 18                  | 0.47     | 0.08                | 0.49       |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 18                  | 0.47     | 0.08                | 0.49       |
| (1,1497) | 1:130:A:ILE:HG21 | 1:131:A:VAL:H    | 18                  | 0.47     | 0.08                | 0.49       |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 18                  | 0.45     | 0.11                | 0.48       |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HG3   | 18                  | 0.45     | 0.11                | 0.48       |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 18                  | 0.37     | 0.09                | 0.38       |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 18                  | 0.37     | 0.09                | 0.38       |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 18                  | 0.37     | 0.09                | 0.38       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 18                  | 0.25     | 0.03                | 0.25       |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 18                  | 0.25     | 0.08                | 0.24       |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 18                  | 0.23     | 0.06                | 0.23       |
| (1,165)  | 1:77:A:ILE:H     | 1:78:A:THR:HG23  | 18                  | 0.23     | 0.06                | 0.23       |
| (1,165)  | 1:77:A:ILE:H     | 1:78:A:THR:HG21  | 18                  | 0.23     | 0.06                | 0.23       |
| (1,165)  | 1:77:A:ILE:H     | 1:78:A:THR:HG22  | 18                  | 0.23     | 0.06                | 0.23       |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HB3  | 18                  | 0.2      | 0.08                | 0.16       |
| (1,1659) | 1:104:A:ILE:HG23 | 1:143:A:TRP:HA   | 18                  | 0.2      | 0.08                | 0.16       |
| (1,1659) | 1:104:A:ILE:HG23 | 1:143:A:TRP:HB3  | 18                  | 0.2      | 0.08                | 0.16       |
| (1,1659) | 1:104:A:ILE:HG22 | 1:143:A:TRP:HB3  | 18                  | 0.2      | 0.08                | 0.16       |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HA   | 18                  | 0.2      | 0.08                | 0.16       |
| (1,1659) | 1:104:A:ILE:HG22 | 1:143:A:TRP:HA   | 18                  | 0.2      | 0.08                | 0.16       |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1  | 17                  | 1.59     | 0.35                | 1.63       |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 17                  | 0.99     | 0.18                | 1.02       |
| (1,1514) | 1:147:A:ILE:HD12 | 1:157:A:VAL:H    | 17                  | 0.94     | 0.39                | 1.0        |
| (1,1514) | 1:147:A:ILE:HD13 | 1:157:A:VAL:H    | 17                  | 0.94     | 0.39                | 1.0        |
| (1,1514) | 1:147:A:ILE:HD11 | 1:157:A:VAL:H    | 17                  | 0.94     | 0.39                | 1.0        |
| (1,1956) | 1:69:A:LEU:HD13  | 1:69:A:LEU:HA    | 17                  | 0.69     | 0.15                | 0.75       |
| (1,1956) | 1:69:A:LEU:HD11  | 1:69:A:LEU:HA    | 17                  | 0.69     | 0.15                | 0.75       |
| (1,1956) | 1:69:A:LEU:HD12  | 1:150:A:HIS:HB3  | 17                  | 0.69     | 0.15                | 0.75       |
| (1,1956) | 1:69:A:LEU:HD12  | 1:69:A:LEU:HA    | 17                  | 0.69     | 0.15                | 0.75       |
| (1,1956) | 1:69:A:LEU:HD11  | 1:150:A:HIS:HB3  | 17                  | 0.69     | 0.15                | 0.75       |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD23 | 17                  | 0.4      | 0.17                | 0.4        |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 17                  | 0.4      | 0.17                | 0.4        |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD21 | 17                  | 0.4      | 0.17                | 0.4        |
| (1,368)  | 1:122:A:LEU:H    | 1:122:A:LEU:HD13 | 17                  | 0.4      | 0.17                | 0.4        |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG22 | 17                  | 0.38     | 0.11                | 0.36       |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 17                  | 0.38     | 0.11                | 0.36       |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG21 | 17                  | 0.38     | 0.11                | 0.36       |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 17                  | 0.33     | 0.14                | 0.3        |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 17                  | 0.33     | 0.14                | 0.3        |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 17                  | 0.33     | 0.14                | 0.3        |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG11  | 17                  | 0.33     | 0.14                | 0.3        |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG12  | 17                  | 0.33     | 0.14                | 0.3        |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG13  | 17                  | 0.33     | 0.14                | 0.3        |
| (1,1702) | 1:99:A:LEU:HD23  | 1:93:A:TYR:HA    | 17                  | 0.29     | 0.1                 | 0.27       |
| (1,1702) | 1:99:A:LEU:HD21  | 1:93:A:TYR:HA    | 17                  | 0.29     | 0.1                 | 0.27       |
| (1,1702) | 1:99:A:LEU:HD22  | 1:93:A:TYR:HA    | 17                  | 0.29     | 0.1                 | 0.27       |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 17                  | 0.28     | 0.06                | 0.29       |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD22 | 17                  | 0.28     | 0.06                | 0.29       |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD21 | 17                  | 0.28     | 0.06                | 0.29       |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 17                  | 0.2      | 0.05                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1983) | 1:77:A:ILE:HD11  | 1:125:A:SER:H    | 17                  | 0.2      | 0.05                | 0.2        |
| (1,1983) | 1:77:A:ILE:HD12  | 1:125:A:SER:H    | 17                  | 0.2      | 0.05                | 0.2        |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 17                  | 0.19     | 0.07                | 0.19       |
| (1,1557) | 1:147:A:ILE:HD12 | 1:143:A:TRP:HB2  | 16                  | 1.17     | 0.33                | 1.18       |
| (1,1557) | 1:147:A:ILE:HD11 | 1:144:A:LYS:HE3  | 16                  | 1.17     | 0.33                | 1.18       |
| (1,1557) | 1:147:A:ILE:HD13 | 1:144:A:LYS:HE2  | 16                  | 1.17     | 0.33                | 1.18       |
| (1,1557) | 1:147:A:ILE:HD11 | 1:143:A:TRP:HB2  | 16                  | 1.17     | 0.33                | 1.18       |
| (1,1557) | 1:147:A:ILE:HD11 | 1:144:A:LYS:HE2  | 16                  | 1.17     | 0.33                | 1.18       |
| (1,1557) | 1:147:A:ILE:HD12 | 1:144:A:LYS:HE2  | 16                  | 1.17     | 0.33                | 1.18       |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG12 | 16                  | 0.85     | 0.22                | 0.86       |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG13 | 16                  | 0.85     | 0.22                | 0.86       |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG11 | 16                  | 0.85     | 0.22                | 0.86       |
| (1,112)  | 1:87:A:SER:H     | 1:130:A:ILE:HD11 | 16                  | 0.85     | 0.22                | 0.86       |
| (1,112)  | 1:87:A:SER:H     | 1:130:A:ILE:HD12 | 16                  | 0.85     | 0.22                | 0.86       |
| (1,1400) | 1:99:A:LEU:HD11  | 1:98:A:GLU:HB3   | 16                  | 0.83     | 0.3                 | 0.85       |
| (1,1400) | 1:99:A:LEU:HD13  | 1:149:A:GLU:HG3  | 16                  | 0.83     | 0.3                 | 0.85       |
| (1,1400) | 1:99:A:LEU:HD13  | 1:98:A:GLU:HB3   | 16                  | 0.83     | 0.3                 | 0.85       |
| (1,1400) | 1:99:A:LEU:HD12  | 1:98:A:GLU:HB3   | 16                  | 0.83     | 0.3                 | 0.85       |
| (1,1400) | 1:99:A:LEU:HD12  | 1:149:A:GLU:HG3  | 16                  | 0.83     | 0.3                 | 0.85       |
| (1,1668) | 1:140:A:THR:HG22 | 1:140:A:THR:H    | 16                  | 0.66     | 0.11                | 0.7        |
| (1,1668) | 1:140:A:THR:HG21 | 1:140:A:THR:H    | 16                  | 0.66     | 0.11                | 0.7        |
| (1,1668) | 1:172:A:THR:HG21 | 1:172:A:THR:H    | 16                  | 0.66     | 0.11                | 0.7        |
| (1,1668) | 1:140:A:THR:HG23 | 1:140:A:THR:H    | 16                  | 0.66     | 0.11                | 0.7        |
| (1,1668) | 1:172:A:THR:HG23 | 1:172:A:THR:H    | 16                  | 0.66     | 0.11                | 0.7        |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE3  | 16                  | 0.59     | 0.16                | 0.54       |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE2  | 16                  | 0.59     | 0.16                | 0.54       |
| (1,1426) | 1:117:A:LYS:HB2  | 1:117:A:LYS:HE3  | 16                  | 0.59     | 0.16                | 0.54       |
| (1,1843) | 1:147:A:ILE:HD11 | 1:102:A:VAL:HB   | 16                  | 0.39     | 0.16                | 0.39       |
| (1,1843) | 1:147:A:ILE:HD12 | 1:102:A:VAL:HB   | 16                  | 0.39     | 0.16                | 0.39       |
| (1,1843) | 1:147:A:ILE:HD13 | 1:144:A:LYS:HG3  | 16                  | 0.39     | 0.16                | 0.39       |
| (1,1843) | 1:147:A:ILE:HD11 | 1:144:A:LYS:HG3  | 16                  | 0.39     | 0.16                | 0.39       |
| (1,1843) | 1:147:A:ILE:HD13 | 1:102:A:VAL:HB   | 16                  | 0.39     | 0.16                | 0.39       |
| (1,1843) | 1:147:A:ILE:HD12 | 1:144:A:LYS:HG3  | 16                  | 0.39     | 0.16                | 0.39       |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 16                  | 0.37     | 0.1                 | 0.42       |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 16                  | 0.37     | 0.1                 | 0.42       |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 16                  | 0.37     | 0.1                 | 0.42       |
| (1,1645) | 1:108:A:ILE:HG23 | 1:84:A:PRO:HD2   | 16                  | 0.35     | 0.16                | 0.36       |
| (1,1645) | 1:108:A:ILE:HG22 | 1:84:A:PRO:HD2   | 16                  | 0.35     | 0.16                | 0.36       |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 16                  | 0.35     | 0.16                | 0.36       |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD23 | 16                  | 0.34     | 0.11                | 0.38       |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD22 | 16                  | 0.34     | 0.11                | 0.38       |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD21 | 16                  | 0.34     | 0.11                | 0.38       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG23 | 16                  | 0.26     | 0.06                | 0.26       |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG21 | 16                  | 0.26     | 0.06                | 0.26       |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG22 | 16                  | 0.26     | 0.06                | 0.26       |
| (1,1909) | 1:170:A:LYS:HA   | 1:171:A:VAL:HG13 | 16                  | 0.26     | 0.06                | 0.26       |
| (1,1909) | 1:170:A:LYS:HA   | 1:171:A:VAL:HG12 | 16                  | 0.26     | 0.06                | 0.26       |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB3   | 16                  | 0.23     | 0.06                | 0.24       |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB2   | 16                  | 0.23     | 0.06                | 0.24       |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB1   | 16                  | 0.23     | 0.06                | 0.24       |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 16                  | 0.18     | 0.04                | 0.17       |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG2   | 16                  | 0.18     | 0.04                | 0.17       |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 16                  | 0.18     | 0.04                | 0.17       |
| (1,1950) | 1:73:A:GLU:HG2   | 1:74:A:LEU:H     | 16                  | 0.18     | 0.04                | 0.17       |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 15                  | 0.53     | 0.27                | 0.58       |
| (1,85)   | 1:125:A:SER:H    | 1:95:A:LYS:HB3   | 15                  | 0.53     | 0.27                | 0.58       |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG21 | 15                  | 0.46     | 0.22                | 0.42       |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG22 | 15                  | 0.46     | 0.22                | 0.42       |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG23 | 15                  | 0.46     | 0.22                | 0.42       |
| (1,2873) | 1:150:A:HIS:HE1  | 1:153:A:VAL:HG21 | 15                  | 0.46     | 0.22                | 0.42       |
| (1,1861) | 1:104:A:ILE:HD13 | 1:140:A:THR:H    | 15                  | 0.35     | 0.14                | 0.37       |
| (1,1861) | 1:104:A:ILE:HD11 | 1:140:A:THR:H    | 15                  | 0.35     | 0.14                | 0.37       |
| (1,1861) | 1:104:A:ILE:HD12 | 1:140:A:THR:H    | 15                  | 0.35     | 0.14                | 0.37       |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 15                  | 0.34     | 0.08                | 0.37       |
| (1,12)   | 1:75:A:LEU:H     | 1:76:A:PRO:HG3   | 15                  | 0.26     | 0.06                | 0.28       |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 15                  | 0.26     | 0.06                | 0.28       |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 15                  | 0.25     | 0.07                | 0.23       |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD13  | 15                  | 0.22     | 0.1                 | 0.21       |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD11  | 15                  | 0.22     | 0.1                 | 0.21       |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD12  | 15                  | 0.22     | 0.1                 | 0.21       |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG12  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG12  | 1:89:A:VAL:HG13  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG12  | 1:89:A:VAL:HG22  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:131:A:VAL:HG23 | 1:89:A:VAL:HG12  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:131:A:VAL:HG22 | 1:89:A:VAL:HG13  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG11  | 1:89:A:VAL:HG21  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG22  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG12  | 1:89:A:VAL:HG21  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG11  | 1:89:A:VAL:HG11  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG13  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG11  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG12  | 1:89:A:VAL:HG23  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG21  | 14                  | 0.78     | 0.36                | 0.79       |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD13 | 14                  | 0.39     | 0.04                | 0.4        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD12 | 14                  | 0.39     | 0.04                | 0.4        |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD11 | 14                  | 0.39     | 0.04                | 0.4        |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 14                  | 0.35     | 0.16                | 0.38       |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 14                  | 0.31     | 0.09                | 0.32       |
| (1,1877) | 1:112:A:VAL:HA   | 1:90:A:TYR:HB2   | 14                  | 0.31     | 0.09                | 0.32       |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 14                  | 0.22     | 0.08                | 0.19       |
| (1,1962) | 1:162:A:LYS:HE3  | 1:159:A:PRO:HA   | 14                  | 0.22     | 0.09                | 0.26       |
| (1,1962) | 1:162:A:LYS:HE2  | 1:159:A:PRO:HA   | 14                  | 0.22     | 0.09                | 0.26       |
| (1,1392) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HD1   | 14                  | 0.21     | 0.07                | 0.18       |
| (1,1392) | 1:126:A:VAL:HG23 | 1:90:A:TYR:HD1   | 14                  | 0.21     | 0.07                | 0.18       |
| (1,1392) | 1:126:A:VAL:HG22 | 1:90:A:TYR:HD1   | 14                  | 0.21     | 0.07                | 0.18       |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG21 | 14                  | 0.21     | 0.07                | 0.18       |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG23 | 14                  | 0.21     | 0.07                | 0.18       |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG22 | 14                  | 0.21     | 0.07                | 0.18       |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 14                  | 0.18     | 0.04                | 0.18       |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 14                  | 0.18     | 0.04                | 0.18       |
| (1,1377) | 1:89:A:VAL:HG11  | 1:66:A:VAL:HG11  | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG13  | 1:131:A:VAL:HG11 | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG11  | 1:131:A:VAL:HG11 | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG23  | 1:131:A:VAL:HG11 | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG22  | 1:131:A:VAL:HG12 | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG13  | 1:139:A:LEU:HD21 | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG23  | 1:139:A:LEU:HD21 | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG13  | 1:131:A:VAL:HG12 | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG11  | 1:66:A:VAL:HG13  | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1377) | 1:89:A:VAL:HG21  | 1:139:A:LEU:HD22 | 13                  | 0.72     | 0.36                | 0.85       |
| (1,1420) | 1:87:A:SER:HB3   | 1:106:A:ARG:HB2  | 13                  | 0.66     | 0.21                | 0.62       |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD3  | 13                  | 0.66     | 0.21                | 0.62       |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD2  | 13                  | 0.66     | 0.21                | 0.62       |
| (1,1420) | 1:87:A:SER:HB3   | 1:106:A:ARG:HG2  | 13                  | 0.66     | 0.21                | 0.62       |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD11 | 13                  | 0.41     | 0.19                | 0.48       |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD12 | 13                  | 0.41     | 0.19                | 0.48       |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD13 | 13                  | 0.41     | 0.19                | 0.48       |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD21 | 13                  | 0.41     | 0.19                | 0.48       |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD22 | 13                  | 0.41     | 0.19                | 0.48       |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD23 | 13                  | 0.41     | 0.19                | 0.48       |
| (1,2799) | 1:93:A:TYR:HE1   | 1:69:A:LEU:HD13  | 13                  | 0.39     | 0.19                | 0.33       |
| (1,2799) | 1:93:A:TYR:HE2   | 1:69:A:LEU:HD13  | 13                  | 0.39     | 0.19                | 0.33       |
| (1,2799) | 1:93:A:TYR:HE2   | 1:69:A:LEU:HD12  | 13                  | 0.39     | 0.19                | 0.33       |
| (1,2799) | 1:93:A:TYR:HE1   | 1:69:A:LEU:HD12  | 13                  | 0.39     | 0.19                | 0.33       |
| (1,2799) | 1:93:A:TYR:HE1   | 1:74:A:LEU:HD22  | 13                  | 0.39     | 0.19                | 0.33       |
| (1,2799) | 1:93:A:TYR:HE1   | 1:74:A:LEU:HD23  | 13                  | 0.39     | 0.19                | 0.33       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2799) | 1:93:A:TYR:HE1   | 1:69:A:LEU:HD11  | 13                  | 0.39     | 0.19                | 0.33       |
| (1,2799) | 1:93:A:TYR:HE2   | 1:74:A:LEU:HD22  | 13                  | 0.39     | 0.19                | 0.33       |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 13                  | 0.27     | 0.15                | 0.19       |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB3  | 13                  | 0.27     | 0.15                | 0.19       |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB2  | 13                  | 0.27     | 0.15                | 0.19       |
| (1,1901) | 1:77:A:ILE:HA    | 1:77:A:ILE:HG13  | 13                  | 0.27     | 0.15                | 0.19       |
| (1,1535) | 1:75:A:LEU:HD22  | 1:76:A:PRO:HD2   | 13                  | 0.25     | 0.07                | 0.28       |
| (1,1535) | 1:75:A:LEU:HD21  | 1:76:A:PRO:HD2   | 13                  | 0.25     | 0.07                | 0.28       |
| (1,1535) | 1:75:A:LEU:HD23  | 1:76:A:PRO:HD2   | 13                  | 0.25     | 0.07                | 0.28       |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG22  | 13                  | 0.22     | 0.11                | 0.19       |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG23  | 13                  | 0.22     | 0.11                | 0.19       |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG21  | 13                  | 0.22     | 0.11                | 0.19       |
| (1,1881) | 1:169:A:VAL:HG23 | 1:168:A:PHE:H    | 13                  | 0.21     | 0.06                | 0.2        |
| (1,1881) | 1:169:A:VAL:HG22 | 1:168:A:PHE:H    | 13                  | 0.21     | 0.06                | 0.2        |
| (1,1881) | 1:169:A:VAL:HG21 | 1:168:A:PHE:H    | 13                  | 0.21     | 0.06                | 0.2        |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB2   | 13                  | 0.21     | 0.11                | 0.15       |
| (1,2795) | 1:93:A:TYR:HD2   | 1:91:A:ALA:HB3   | 13                  | 0.21     | 0.11                | 0.15       |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB1   | 13                  | 0.21     | 0.11                | 0.15       |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB3   | 13                  | 0.21     | 0.11                | 0.15       |
| (1,2795) | 1:93:A:TYR:HD2   | 1:91:A:ALA:HB2   | 13                  | 0.21     | 0.11                | 0.15       |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 13                  | 0.13     | 0.01                | 0.13       |
| (1,2011) | 1:151:A:ILE:HD11 | 1:157:A:VAL:H    | 12                  | 0.93     | 0.33                | 0.9        |
| (1,2011) | 1:151:A:ILE:HD13 | 1:157:A:VAL:H    | 12                  | 0.93     | 0.33                | 0.9        |
| (1,2011) | 1:151:A:ILE:HD13 | 1:156:A:LYS:H    | 12                  | 0.93     | 0.33                | 0.9        |
| (1,2011) | 1:151:A:ILE:HD12 | 1:157:A:VAL:H    | 12                  | 0.93     | 0.33                | 0.9        |
| (1,363)  | 1:155:A:GLY:H    | 1:154:A:THR:HG23 | 12                  | 0.68     | 0.14                | 0.68       |
| (1,363)  | 1:155:A:GLY:H    | 1:154:A:THR:HG22 | 12                  | 0.68     | 0.14                | 0.68       |
| (1,363)  | 1:155:A:GLY:H    | 1:153:A:VAL:HG22 | 12                  | 0.68     | 0.14                | 0.68       |
| (1,363)  | 1:155:A:GLY:H    | 1:153:A:VAL:HG21 | 12                  | 0.68     | 0.14                | 0.68       |
| (1,363)  | 1:155:A:GLY:H    | 1:153:A:VAL:HG23 | 12                  | 0.68     | 0.14                | 0.68       |
| (1,1807) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 12                  | 0.67     | 0.09                | 0.7        |
| (1,1807) | 1:154:A:THR:HG22 | 1:155:A:GLY:H    | 12                  | 0.67     | 0.09                | 0.7        |
| (1,1807) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 12                  | 0.67     | 0.09                | 0.7        |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG2  | 12                  | 0.55     | 0.16                | 0.55       |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG3  | 12                  | 0.55     | 0.16                | 0.55       |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD12 | 12                  | 0.43     | 0.27                | 0.36       |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD11 | 12                  | 0.43     | 0.27                | 0.36       |
| (1,99)   | 1:160:A:GLY:H    | 1:157:A:VAL:HG13 | 12                  | 0.43     | 0.27                | 0.36       |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD13 | 12                  | 0.43     | 0.27                | 0.36       |
| (1,99)   | 1:160:A:GLY:H    | 1:157:A:VAL:HG23 | 12                  | 0.43     | 0.27                | 0.36       |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 12                  | 0.41     | 0.17                | 0.43       |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 12                  | 0.41     | 0.15                | 0.43       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 12                  | 0.41     | 0.15                | 0.43       |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 12                  | 0.41     | 0.15                | 0.43       |
| (1,1506) | 1:170:A:LYS:HE2  | 1:171:A:VAL:H    | 12                  | 0.4      | 0.2                 | 0.37       |
| (1,1506) | 1:156:A:LYS:HE3  | 1:157:A:VAL:H    | 12                  | 0.4      | 0.2                 | 0.37       |
| (1,1506) | 1:156:A:LYS:HE2  | 1:157:A:VAL:H    | 12                  | 0.4      | 0.2                 | 0.37       |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 12                  | 0.4      | 0.17                | 0.48       |
| (1,1402) | 1:112:A:VAL:HA   | 1:90:A:TYR:HE1   | 12                  | 0.37     | 0.19                | 0.38       |
| (1,1402) | 1:112:A:VAL:HA   | 1:115:A:HIS:HD2  | 12                  | 0.37     | 0.19                | 0.38       |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 12                  | 0.27     | 0.03                | 0.29       |
| (1,2820) | 1:168:A:PHE:HZ   | 1:92:A:VAL:HG11  | 12                  | 0.27     | 0.03                | 0.29       |
| (1,1551) | 1:99:A:LEU:HD23  | 1:103:A:GLY:H    | 12                  | 0.27     | 0.11                | 0.23       |
| (1,1551) | 1:99:A:LEU:HD22  | 1:103:A:GLY:H    | 12                  | 0.27     | 0.11                | 0.23       |
| (1,1551) | 1:99:A:LEU:HD21  | 1:103:A:GLY:H    | 12                  | 0.27     | 0.11                | 0.23       |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD22 | 12                  | 0.24     | 0.19                | 0.18       |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD23 | 12                  | 0.24     | 0.19                | 0.18       |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD21 | 12                  | 0.24     | 0.19                | 0.18       |
| (1,1511) | 1:128:A:VAL:HG13 | 1:90:A:TYR:H     | 12                  | 0.19     | 0.07                | 0.2        |
| (1,1511) | 1:128:A:VAL:HG11 | 1:90:A:TYR:H     | 12                  | 0.19     | 0.07                | 0.2        |
| (1,1511) | 1:128:A:VAL:HG12 | 1:90:A:TYR:H     | 12                  | 0.19     | 0.07                | 0.2        |
| (1,1464) | 1:152:A:LYS:HA   | 1:152:A:LYS:HG3  | 12                  | 0.19     | 0.04                | 0.18       |
| (1,1464) | 1:136:A:LYS:HA   | 1:136:A:LYS:HG3  | 12                  | 0.19     | 0.04                | 0.18       |
| (1,1464) | 1:136:A:LYS:HA   | 1:136:A:LYS:HG2  | 12                  | 0.19     | 0.04                | 0.18       |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HD12 | 11                  | 0.29     | 0.14                | 0.28       |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG22 | 11                  | 0.29     | 0.14                | 0.28       |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG23 | 11                  | 0.29     | 0.14                | 0.28       |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG21 | 11                  | 0.29     | 0.14                | 0.28       |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HD11 | 11                  | 0.29     | 0.14                | 0.28       |
| (1,1454) | 1:89:A:VAL:HG11  | 1:139:A:LEU:HG   | 10                  | 1.49     | 0.17                | 1.51       |
| (1,1454) | 1:89:A:VAL:HG13  | 1:139:A:LEU:HG   | 10                  | 1.49     | 0.17                | 1.51       |
| (1,1454) | 1:89:A:VAL:HG21  | 1:139:A:LEU:HB2  | 10                  | 1.49     | 0.17                | 1.51       |
| (1,1454) | 1:89:A:VAL:HG22  | 1:139:A:LEU:HB2  | 10                  | 1.49     | 0.17                | 1.51       |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG12  | 10                  | 0.98     | 0.33                | 1.03       |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG11  | 10                  | 0.98     | 0.33                | 1.03       |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG13  | 10                  | 0.98     | 0.33                | 1.03       |
| (1,1433) | 1:136:A:LYS:HD2  | 1:104:A:ILE:HG23 | 10                  | 0.79     | 0.37                | 0.82       |
| (1,1433) | 1:170:A:LYS:HD2  | 1:167:A:THR:HG21 | 10                  | 0.79     | 0.37                | 0.82       |
| (1,1433) | 1:170:A:LYS:HD2  | 1:167:A:THR:HG23 | 10                  | 0.79     | 0.37                | 0.82       |
| (1,1433) | 1:170:A:LYS:HD2  | 1:167:A:THR:HG22 | 10                  | 0.79     | 0.37                | 0.82       |
| (1,1433) | 1:117:A:LYS:HD3  | 1:116:A:LEU:HD21 | 10                  | 0.79     | 0.37                | 0.82       |
| (1,1433) | 1:136:A:LYS:HD2  | 1:104:A:ILE:HG22 | 10                  | 0.79     | 0.37                | 0.82       |
| (1,1433) | 1:117:A:LYS:HD3  | 1:116:A:LEU:HD23 | 10                  | 0.79     | 0.37                | 0.82       |
| (1,1433) | 1:136:A:LYS:HD2  | 1:104:A:ILE:HG21 | 10                  | 0.79     | 0.37                | 0.82       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1433) | 1:117:A:LYS:HD3  | 1:116:A:LEU:HD22 | 10                  | 0.79     | 0.37                | 0.82       |
| (1,1676) | 1:99:A:LEU:HD21  | 1:126:A:VAL:HB   | 10                  | 0.79     | 0.45                | 0.88       |
| (1,1676) | 1:99:A:LEU:HD23  | 1:126:A:VAL:HB   | 10                  | 0.79     | 0.45                | 0.88       |
| (1,1676) | 1:69:A:LEU:HD23  | 1:149:A:GLU:HB3  | 10                  | 0.79     | 0.45                | 0.88       |
| (1,1676) | 1:69:A:LEU:HD22  | 1:149:A:GLU:HB3  | 10                  | 0.79     | 0.45                | 0.88       |
| (1,1676) | 1:69:A:LEU:HD21  | 1:149:A:GLU:HB3  | 10                  | 0.79     | 0.45                | 0.88       |
| (1,1676) | 1:99:A:LEU:HD22  | 1:126:A:VAL:HB   | 10                  | 0.79     | 0.45                | 0.88       |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG21 | 10                  | 0.62     | 0.2                 | 0.74       |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG22 | 10                  | 0.62     | 0.2                 | 0.74       |
| (1,159)  | 1:153:A:VAL:H    | 1:154:A:THR:HG22 | 10                  | 0.62     | 0.2                 | 0.74       |
| (1,159)  | 1:153:A:VAL:H    | 1:154:A:THR:HG21 | 10                  | 0.62     | 0.2                 | 0.74       |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG23 | 10                  | 0.62     | 0.2                 | 0.74       |
| (1,1382) | 1:170:A:LYS:HB3  | 1:170:A:LYS:HE3  | 10                  | 0.6      | 0.05                | 0.6        |
| (1,1382) | 1:170:A:LYS:HB2  | 1:170:A:LYS:HE2  | 10                  | 0.6      | 0.05                | 0.6        |
| (1,1382) | 1:117:A:LYS:HB3  | 1:117:A:LYS:HE3  | 10                  | 0.6      | 0.05                | 0.6        |
| (1,1382) | 1:170:A:LYS:HB2  | 1:170:A:LYS:HE3  | 10                  | 0.6      | 0.05                | 0.6        |
| (1,1395) | 1:153:A:VAL:HG11 | 1:150:A:HIS:HA   | 10                  | 0.6      | 0.22                | 0.51       |
| (1,1395) | 1:153:A:VAL:HG12 | 1:150:A:HIS:HA   | 10                  | 0.6      | 0.22                | 0.51       |
| (1,1395) | 1:153:A:VAL:HG13 | 1:150:A:HIS:HA   | 10                  | 0.6      | 0.22                | 0.51       |
| (1,1510) | 1:115:A:HIS:HB3  | 1:167:A:THR:HG21 | 10                  | 0.51     | 0.19                | 0.48       |
| (1,1510) | 1:115:A:HIS:HB3  | 1:116:A:LEU:HD23 | 10                  | 0.51     | 0.19                | 0.48       |
| (1,1510) | 1:115:A:HIS:HB3  | 1:116:A:LEU:HD22 | 10                  | 0.51     | 0.19                | 0.48       |
| (1,1510) | 1:115:A:HIS:HB3  | 1:167:A:THR:HG23 | 10                  | 0.51     | 0.19                | 0.48       |
| (1,1510) | 1:115:A:HIS:HB3  | 1:167:A:THR:HG22 | 10                  | 0.51     | 0.19                | 0.48       |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE3   | 10                  | 0.45     | 0.1                 | 0.47       |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE2   | 10                  | 0.45     | 0.1                 | 0.47       |
| (1,101)  | 1:89:A:VAL:H     | 1:139:A:LEU:HD21 | 10                  | 0.43     | 0.14                | 0.42       |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG13 | 10                  | 0.43     | 0.14                | 0.42       |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG12 | 10                  | 0.43     | 0.14                | 0.42       |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG11 | 10                  | 0.43     | 0.14                | 0.42       |
| (1,1422) | 1:145:A:LEU:HD21 | 1:145:A:LEU:H    | 10                  | 0.4      | 0.04                | 0.4        |
| (1,1422) | 1:145:A:LEU:HD23 | 1:145:A:LEU:H    | 10                  | 0.4      | 0.04                | 0.4        |
| (1,1422) | 1:145:A:LEU:HD22 | 1:145:A:LEU:H    | 10                  | 0.4      | 0.04                | 0.4        |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG23 | 10                  | 0.35     | 0.05                | 0.36       |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG22 | 10                  | 0.35     | 0.05                | 0.36       |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG21 | 10                  | 0.35     | 0.05                | 0.36       |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE2  | 10                  | 0.33     | 0.13                | 0.32       |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE3  | 10                  | 0.33     | 0.13                | 0.32       |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 10                  | 0.32     | 0.14                | 0.29       |
| (1,1508) | 1:169:A:VAL:HB   | 1:170:A:LYS:HD3  | 10                  | 0.32     | 0.14                | 0.29       |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 10                  | 0.32     | 0.02                | 0.32       |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD21 | 10                  | 0.29     | 0.1                 | 0.26       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD23 | 10                  | 0.29     | 0.1                 | 0.26       |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD22 | 10                  | 0.29     | 0.1                 | 0.26       |
| (1,1844) | 1:108:A:ILE:HA   | 1:110:A:ALA:HB2  | 10                  | 0.27     | 0.1                 | 0.34       |
| (1,1844) | 1:108:A:ILE:HA   | 1:110:A:ALA:HB3  | 10                  | 0.27     | 0.1                 | 0.34       |
| (1,1844) | 1:108:A:ILE:HA   | 1:109:A:ALA:HB2  | 10                  | 0.27     | 0.1                 | 0.34       |
| (1,1844) | 1:108:A:ILE:HA   | 1:109:A:ALA:HB1  | 10                  | 0.27     | 0.1                 | 0.34       |
| (1,1844) | 1:108:A:ILE:HA   | 1:110:A:ALA:HB1  | 10                  | 0.27     | 0.1                 | 0.34       |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 10                  | 0.16     | 0.05                | 0.15       |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 9                   | 0.6      | 0.1                 | 0.57       |
| (1,1396) | 1:83:A:ILE:HG22  | 1:90:A:TYR:HD2   | 9                   | 0.33     | 0.11                | 0.28       |
| (1,1396) | 1:83:A:ILE:HG21  | 1:90:A:TYR:HD2   | 9                   | 0.33     | 0.11                | 0.28       |
| (1,1396) | 1:83:A:ILE:HG23  | 1:90:A:TYR:HD2   | 9                   | 0.33     | 0.11                | 0.28       |
| (1,1396) | 1:83:A:ILE:HG21  | 1:90:A:TYR:HD1   | 9                   | 0.33     | 0.11                | 0.28       |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 9                   | 0.33     | 0.24                | 0.21       |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD12 | 9                   | 0.28     | 0.12                | 0.24       |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD11 | 9                   | 0.28     | 0.12                | 0.24       |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD13 | 9                   | 0.28     | 0.12                | 0.24       |
| (1,1448) | 1:156:A:LYS:HD2  | 1:156:A:LYS:H    | 9                   | 0.25     | 0.11                | 0.22       |
| (1,1448) | 1:156:A:LYS:HD3  | 1:156:A:LYS:H    | 9                   | 0.25     | 0.11                | 0.22       |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,2026) | 1:109:A:ALA:HB3  | 1:83:A:ILE:HG22  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,2026) | 1:109:A:ALA:HB1  | 1:83:A:ILE:HG22  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,2026) | 1:109:A:ALA:HB2  | 1:83:A:ILE:HG22  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,2026) | 1:109:A:ALA:HB1  | 1:83:A:ILE:HG21  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,2026) | 1:109:A:ALA:HB2  | 1:83:A:ILE:HG23  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,2026) | 1:109:A:ALA:HB2  | 1:83:A:ILE:HG21  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,2026) | 1:109:A:ALA:HB3  | 1:83:A:ILE:HG23  | 9                   | 0.23     | 0.07                | 0.24       |
| (1,148)  | 1:91:A:ALA:H     | 1:126:A:VAL:HB   | 9                   | 0.17     | 0.05                | 0.14       |
| (1,148)  | 1:91:A:ALA:H     | 1:128:A:VAL:HB   | 9                   | 0.17     | 0.05                | 0.14       |
| (1,1566) | 1:119:A:VAL:HG23 | 1:167:A:THR:HG22 | 8                   | 0.5      | 0.24                | 0.53       |
| (1,1566) | 1:119:A:VAL:HG21 | 1:167:A:THR:HG23 | 8                   | 0.5      | 0.24                | 0.53       |
| (1,1566) | 1:119:A:VAL:HG23 | 1:167:A:THR:HG21 | 8                   | 0.5      | 0.24                | 0.53       |
| (1,1566) | 1:119:A:VAL:HG22 | 1:167:A:THR:HG23 | 8                   | 0.5      | 0.24                | 0.53       |
| (1,1566) | 1:119:A:VAL:HG23 | 1:167:A:THR:HG23 | 8                   | 0.5      | 0.24                | 0.53       |
| (1,1566) | 1:119:A:VAL:HG21 | 1:167:A:THR:HG22 | 8                   | 0.5      | 0.24                | 0.53       |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG13 | 8                   | 0.39     | 0.18                | 0.28       |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG22 | 8                   | 0.39     | 0.18                | 0.28       |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG12 | 8                   | 0.39     | 0.18                | 0.28       |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG21 | 8                   | 0.39     | 0.18                | 0.28       |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG11 | 8                   | 0.39     | 0.18                | 0.28       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG2 | 8                   | 0.39     | 0.17                | 0.41       |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG3 | 8                   | 0.39     | 0.17                | 0.41       |
| (1,90)   | 1:124:A:GLY:H    | 1:92:A:VAL:HG11 | 8                   | 0.32     | 0.15                | 0.3        |
| (1,90)   | 1:124:A:GLY:H    | 1:77:A:ILE:HG13 | 8                   | 0.32     | 0.15                | 0.3        |
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2 | 8                   | 0.25     | 0.09                | 0.26       |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H   | 8                   | 0.24     | 0.03                | 0.24       |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2 | 8                   | 0.24     | 0.06                | 0.22       |
| (1,44)   | 1:160:A:GLY:H    | 1:159:A:PRO:HG2 | 8                   | 0.18     | 0.1                 | 0.12       |
| (1,44)   | 1:160:A:GLY:H    | 1:159:A:PRO:HB2 | 8                   | 0.18     | 0.1                 | 0.12       |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3  | 8                   | 0.15     | 0.02                | 0.14       |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB3 | 8                   | 0.15     | 0.03                | 0.14       |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB3 | 8                   | 0.15     | 0.03                | 0.14       |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB3 | 8                   | 0.15     | 0.03                | 0.14       |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB2 | 8                   | 0.15     | 0.03                | 0.14       |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB2 | 8                   | 0.15     | 0.03                | 0.14       |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB2 | 8                   | 0.15     | 0.03                | 0.14       |
| (1,1487) | 1:126:A:VAL:HA   | 1:92:A:VAL:HB   | 8                   | 0.15     | 0.05                | 0.12       |
| (1,1487) | 1:126:A:VAL:HA   | 1:75:A:LEU:HB2  | 8                   | 0.15     | 0.05                | 0.12       |
| (1,220)  | 1:82:A:SER:H     | 1:82:A:SER:HA   | 8                   | 0.11     | 0.01                | 0.11       |
| (1,1544) | 1:173:A:LEU:HD12 | 1:173:A:LEU:HA  | 7                   | 0.65     | 0.2                 | 0.66       |
| (1,1544) | 1:173:A:LEU:HD11 | 1:173:A:LEU:HA  | 7                   | 0.65     | 0.2                 | 0.66       |
| (1,1544) | 1:173:A:LEU:HD13 | 1:173:A:LEU:HA  | 7                   | 0.65     | 0.2                 | 0.66       |
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE3 | 7                   | 0.55     | 0.12                | 0.55       |
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE2 | 7                   | 0.55     | 0.12                | 0.55       |
| (1,1984) | 1:69:A:LEU:HD11  | 1:151:A:ILE:H   | 7                   | 0.5      | 0.49                | 0.29       |
| (1,1984) | 1:69:A:LEU:HD11  | 1:68:A:SER:H    | 7                   | 0.5      | 0.49                | 0.29       |
| (1,1984) | 1:69:A:LEU:HD13  | 1:151:A:ILE:H   | 7                   | 0.5      | 0.49                | 0.29       |
| (1,1984) | 1:69:A:LEU:HD12  | 1:151:A:ILE:H   | 7                   | 0.5      | 0.49                | 0.29       |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD11 | 7                   | 0.4      | 0.15                | 0.39       |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD12 | 7                   | 0.4      | 0.15                | 0.39       |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD13 | 7                   | 0.4      | 0.15                | 0.39       |
| (1,1681) | 1:156:A:LYS:HG2  | 1:99:A:LEU:HD11 | 7                   | 0.4      | 0.15                | 0.39       |
| (1,1681) | 1:156:A:LYS:HG2  | 1:99:A:LEU:HD12 | 7                   | 0.4      | 0.15                | 0.39       |
| (1,1681) | 1:156:A:LYS:HG2  | 1:99:A:LEU:HD13 | 7                   | 0.4      | 0.15                | 0.39       |
| (1,2025) | 1:144:A:LYS:HE2  | 1:143:A:TRP:HZ3 | 7                   | 0.35     | 0.11                | 0.29       |
| (1,2025) | 1:144:A:LYS:HE3  | 1:143:A:TRP:HZ3 | 7                   | 0.35     | 0.11                | 0.29       |
| (1,1565) | 1:167:A:THR:HA   | 1:168:A:PHE:HB2 | 7                   | 0.31     | 0.03                | 0.31       |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG23 | 7                   | 0.3      | 0.17                | 0.33       |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG22 | 7                   | 0.3      | 0.17                | 0.33       |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG21 | 7                   | 0.3      | 0.17                | 0.33       |
| (1,1383) | 1:80:A:ALA:HB3   | 1:83:A:ILE:HG13 | 7                   | 0.27     | 0.1                 | 0.25       |
| (1,1383) | 1:80:A:ALA:HB2   | 1:83:A:ILE:HG13 | 7                   | 0.27     | 0.1                 | 0.25       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1383) | 1:80:A:ALA:HB1   | 1:83:A:ILE:HG13  | 7                   | 0.27     | 0.1                 | 0.25       |
| (1,1862) | 1:144:A:LYS:HE3  | 1:145:A:LEU:H    | 7                   | 0.24     | 0.07                | 0.26       |
| (1,1862) | 1:144:A:LYS:HE2  | 1:145:A:LEU:H    | 7                   | 0.24     | 0.07                | 0.26       |
| (1,1378) | 1:136:A:LYS:HE2  | 1:136:A:LYS:HB2  | 6                   | 0.73     | 0.14                | 0.68       |
| (1,1378) | 1:117:A:LYS:HE3  | 1:117:A:LYS:HB3  | 6                   | 0.73     | 0.14                | 0.68       |
| (1,1378) | 1:136:A:LYS:HE3  | 1:136:A:LYS:HB3  | 6                   | 0.73     | 0.14                | 0.68       |
| (1,1388) | 1:67:A:LYS:HD3   | 1:66:A:VAL:HG11  | 6                   | 0.67     | 0.29                | 0.63       |
| (1,1388) | 1:67:A:LYS:HD3   | 1:66:A:VAL:HG13  | 6                   | 0.67     | 0.29                | 0.63       |
| (1,1388) | 1:95:A:LYS:HD2   | 1:77:A:ILE:HD13  | 6                   | 0.67     | 0.29                | 0.63       |
| (1,2797) | 1:150:A:HIS:HE1  | 1:98:A:GLU:HB3   | 6                   | 0.56     | 0.29                | 0.49       |
| (1,2797) | 1:150:A:HIS:HE1  | 1:153:A:VAL:HB   | 6                   | 0.56     | 0.29                | 0.49       |
| (1,2797) | 1:150:A:HIS:HE1  | 1:98:A:GLU:HG2   | 6                   | 0.56     | 0.29                | 0.49       |
| (1,1494) | 1:172:A:THR:HB   | 1:171:A:VAL:HG13 | 6                   | 0.51     | 0.24                | 0.48       |
| (1,1494) | 1:172:A:THR:HB   | 1:173:A:LEU:HD12 | 6                   | 0.51     | 0.24                | 0.48       |
| (1,1494) | 1:172:A:THR:HB   | 1:171:A:VAL:HG12 | 6                   | 0.51     | 0.24                | 0.48       |
| (1,1494) | 1:172:A:THR:HB   | 1:171:A:VAL:HG22 | 6                   | 0.51     | 0.24                | 0.48       |
| (1,1494) | 1:172:A:THR:HB   | 1:173:A:LEU:HD11 | 6                   | 0.51     | 0.24                | 0.48       |
| (1,1850) | 1:147:A:ILE:HD11 | 1:148:A:GLU:HG3  | 6                   | 0.5      | 0.26                | 0.38       |
| (1,1850) | 1:147:A:ILE:HD12 | 1:148:A:GLU:HG3  | 6                   | 0.5      | 0.26                | 0.38       |
| (1,1850) | 1:147:A:ILE:HD13 | 1:148:A:GLU:HG3  | 6                   | 0.5      | 0.26                | 0.38       |
| (1,63)   | 1:170:A:LYS:H    | 1:166:A:ASN:HB2  | 6                   | 0.46     | 0.25                | 0.34       |
| (1,63)   | 1:170:A:LYS:H    | 1:170:A:LYS:HE3  | 6                   | 0.46     | 0.25                | 0.34       |
| (1,63)   | 1:170:A:LYS:H    | 1:170:A:LYS:HE2  | 6                   | 0.46     | 0.25                | 0.34       |
| (1,25)   | 1:135:A:ASP:H    | 1:134:A:PRO:HG2  | 6                   | 0.44     | 0.13                | 0.48       |
| (1,25)   | 1:135:A:ASP:H    | 1:134:A:PRO:HB2  | 6                   | 0.44     | 0.13                | 0.48       |
| (1,1947) | 1:70:A:THR:HB    | 1:67:A:LYS:HB2   | 6                   | 0.41     | 0.08                | 0.4        |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD11  | 6                   | 0.36     | 0.1                 | 0.34       |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD12  | 6                   | 0.36     | 0.1                 | 0.34       |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD13  | 6                   | 0.36     | 0.1                 | 0.34       |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD11  | 6                   | 0.36     | 0.1                 | 0.34       |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD12  | 6                   | 0.36     | 0.1                 | 0.34       |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD13  | 6                   | 0.36     | 0.1                 | 0.34       |
| (1,351)  | 1:100:A:GLN:HE22 | 1:98:A:GLU:HG3   | 6                   | 0.34     | 0.04                | 0.32       |
| (1,1999) | 1:98:A:GLU:HG3   | 1:100:A:GLN:HE22 | 6                   | 0.34     | 0.04                | 0.32       |
| (1,1953) | 1:83:A:ILE:HG21  | 1:128:A:VAL:HA   | 6                   | 0.34     | 0.18                | 0.29       |
| (1,1953) | 1:130:A:ILE:HG22 | 1:88:A:GLY:HA2   | 6                   | 0.34     | 0.18                | 0.29       |
| (1,1953) | 1:83:A:ILE:HG22  | 1:128:A:VAL:HA   | 6                   | 0.34     | 0.18                | 0.29       |
| (1,1953) | 1:130:A:ILE:HG21 | 1:88:A:GLY:HA2   | 6                   | 0.34     | 0.18                | 0.29       |
| (1,311)  | 1:88:A:GLY:H     | 1:106:A:ARG:HD3  | 6                   | 0.24     | 0.11                | 0.2        |
| (1,311)  | 1:88:A:GLY:H     | 1:106:A:ARG:HD2  | 6                   | 0.24     | 0.11                | 0.2        |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD21 | 6                   | 0.23     | 0.12                | 0.18       |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD22 | 6                   | 0.23     | 0.12                | 0.18       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD23 | 6                   | 0.23     | 0.12                | 0.18       |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD11 | 6                   | 0.23     | 0.12                | 0.18       |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD12 | 6                   | 0.23     | 0.12                | 0.18       |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD13 | 6                   | 0.23     | 0.12                | 0.18       |
| (1,1690) | 1:145:A:LEU:HD21 | 1:67:A:LYS:H     | 6                   | 0.23     | 0.12                | 0.18       |
| (1,1690) | 1:145:A:LEU:HD22 | 1:67:A:LYS:H     | 6                   | 0.23     | 0.12                | 0.18       |
| (1,1690) | 1:145:A:LEU:HD23 | 1:67:A:LYS:H     | 6                   | 0.23     | 0.12                | 0.18       |
| (1,1690) | 1:145:A:LEU:HD11 | 1:67:A:LYS:H     | 6                   | 0.23     | 0.12                | 0.18       |
| (1,1690) | 1:145:A:LEU:HD12 | 1:67:A:LYS:H     | 6                   | 0.23     | 0.12                | 0.18       |
| (1,1690) | 1:145:A:LEU:HD13 | 1:67:A:LYS:H     | 6                   | 0.23     | 0.12                | 0.18       |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG12 | 6                   | 0.23     | 0.08                | 0.26       |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG11 | 6                   | 0.23     | 0.08                | 0.26       |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG13 | 6                   | 0.23     | 0.08                | 0.26       |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG23 | 6                   | 0.19     | 0.09                | 0.16       |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG21 | 6                   | 0.19     | 0.09                | 0.16       |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG12 | 6                   | 0.19     | 0.09                | 0.16       |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG11 | 6                   | 0.19     | 0.09                | 0.16       |
| (1,2656) | 1:86:A:ALA:HB1   | 1:107:A:ASN:HD21 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,2656) | 1:86:A:ALA:HB2   | 1:107:A:ASN:HD21 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,2656) | 1:86:A:ALA:HB3   | 1:107:A:ASN:HD21 | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1390) | 1:152:A:LYS:HE3  | 1:148:A:GLU:HB3  | 5                   | 0.49     | 0.2                 | 0.42       |
| (1,1390) | 1:152:A:LYS:HE2  | 1:148:A:GLU:HB3  | 5                   | 0.49     | 0.2                 | 0.42       |
| (1,1390) | 1:152:A:LYS:HE2  | 1:149:A:GLU:HB3  | 5                   | 0.49     | 0.2                 | 0.42       |
| (1,1456) | 1:157:A:VAL:HG21 | 1:151:A:ILE:HG13 | 5                   | 0.4      | 0.23                | 0.32       |
| (1,1456) | 1:157:A:VAL:HG22 | 1:151:A:ILE:HG13 | 5                   | 0.4      | 0.23                | 0.32       |
| (1,1456) | 1:157:A:VAL:HG23 | 1:151:A:ILE:HG13 | 5                   | 0.4      | 0.23                | 0.32       |
| (1,1456) | 1:157:A:VAL:HG11 | 1:151:A:ILE:HG13 | 5                   | 0.4      | 0.23                | 0.32       |
| (1,1456) | 1:157:A:VAL:HG12 | 1:151:A:ILE:HG13 | 5                   | 0.4      | 0.23                | 0.32       |
| (1,1456) | 1:157:A:VAL:HG13 | 1:151:A:ILE:HG13 | 5                   | 0.4      | 0.23                | 0.32       |
| (1,236)  | 1:156:A:LYS:H    | 1:156:A:LYS:HE3  | 5                   | 0.35     | 0.11                | 0.35       |
| (1,236)  | 1:156:A:LYS:H    | 1:156:A:LYS:HE2  | 5                   | 0.35     | 0.11                | 0.35       |
| (1,302)  | 1:146:A:TRP:HE1  | 1:69:A:LEU:HB3   | 5                   | 0.31     | 0.17                | 0.29       |
| (1,302)  | 1:146:A:TRP:HE1  | 1:69:A:LEU:HD12  | 5                   | 0.31     | 0.17                | 0.29       |
| (1,1539) | 1:69:A:LEU:HD11  | 1:150:A:HIS:HA   | 5                   | 0.3      | 0.23                | 0.22       |
| (1,1539) | 1:69:A:LEU:HD12  | 1:149:A:GLU:HA   | 5                   | 0.3      | 0.23                | 0.22       |
| (1,1539) | 1:69:A:LEU:HD12  | 1:150:A:HIS:HA   | 5                   | 0.3      | 0.23                | 0.22       |
| (1,1539) | 1:69:A:LEU:HD13  | 1:150:A:HIS:HA   | 5                   | 0.3      | 0.23                | 0.22       |
| (1,394)  | 1:121:A:GLU:H    | 1:116:A:LEU:HD23 | 5                   | 0.28     | 0.09                | 0.23       |
| (1,394)  | 1:121:A:GLU:H    | 1:116:A:LEU:HD22 | 5                   | 0.28     | 0.09                | 0.23       |
| (1,243)  | 1:162:A:LYS:H    | 1:162:A:LYS:HE2  | 5                   | 0.27     | 0.07                | 0.29       |
| (1,243)  | 1:162:A:LYS:H    | 1:162:A:LYS:HE3  | 5                   | 0.27     | 0.07                | 0.29       |
| (1,1994) | 1:162:A:LYS:HE2  | 1:162:A:LYS:H    | 5                   | 0.27     | 0.07                | 0.29       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1994) | 1:162:A:LYS:HE3  | 1:162:A:LYS:H    | 5                   | 0.27     | 0.07                | 0.29       |
| (1,9)    | 1:79:A:GLU:H     | 1:77:A:ILE:HA    | 5                   | 0.26     | 0.1                 | 0.26       |
| (1,1948) | 1:87:A:SER:HB3   | 1:131:A:VAL:H    | 5                   | 0.25     | 0.07                | 0.25       |
| (1,1864) | 1:147:A:ILE:HG21 | 1:144:A:LYS:HE3  | 5                   | 0.23     | 0.05                | 0.25       |
| (1,1864) | 1:147:A:ILE:HG22 | 1:144:A:LYS:HE3  | 5                   | 0.23     | 0.05                | 0.25       |
| (1,1864) | 1:147:A:ILE:HG23 | 1:144:A:LYS:HE3  | 5                   | 0.23     | 0.05                | 0.25       |
| (1,1864) | 1:147:A:ILE:HG21 | 1:144:A:LYS:HE2  | 5                   | 0.23     | 0.05                | 0.25       |
| (1,1864) | 1:147:A:ILE:HG22 | 1:144:A:LYS:HE2  | 5                   | 0.23     | 0.05                | 0.25       |
| (1,1864) | 1:147:A:ILE:HG23 | 1:144:A:LYS:HE2  | 5                   | 0.23     | 0.05                | 0.25       |
| (1,7)    | 1:139:A:LEU:H    | 1:138:A:VAL:HG13 | 5                   | 0.2      | 0.08                | 0.16       |
| (1,7)    | 1:139:A:LEU:H    | 1:138:A:VAL:HG11 | 5                   | 0.2      | 0.08                | 0.16       |
| (1,1902) | 1:77:A:ILE:HA    | 1:76:A:PRO:HB3   | 5                   | 0.13     | 0.02                | 0.12       |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG21 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG22 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG23 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG21 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG22 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG23 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG21 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG22 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG23 | 5                   | 0.13     | 0.02                | 0.13       |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG21  | 4                   | 0.48     | 0.05                | 0.5        |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG22  | 4                   | 0.48     | 0.05                | 0.5        |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG23  | 4                   | 0.48     | 0.05                | 0.5        |
| (1,231)  | 1:140:A:THR:H    | 1:136:A:LYS:HE2  | 4                   | 0.36     | 0.07                | 0.4        |
| (1,84)   | 1:72:A:THR:H     | 1:69:A:LEU:HG    | 4                   | 0.34     | 0.16                | 0.3        |
| (1,84)   | 1:72:A:THR:H     | 1:66:A:VAL:HG12  | 4                   | 0.34     | 0.16                | 0.3        |
| (1,84)   | 1:72:A:THR:H     | 1:66:A:VAL:HG11  | 4                   | 0.34     | 0.16                | 0.3        |
| (1,1801) | 1:159:A:PRO:HG3  | 1:162:A:LYS:HE2  | 4                   | 0.32     | 0.14                | 0.24       |
| (1,1801) | 1:159:A:PRO:HG3  | 1:162:A:LYS:HE3  | 4                   | 0.32     | 0.14                | 0.24       |
| (1,1504) | 1:147:A:ILE:HD11 | 1:157:A:VAL:HG13 | 4                   | 0.31     | 0.18                | 0.22       |
| (1,1504) | 1:147:A:ILE:HD12 | 1:102:A:VAL:HG23 | 4                   | 0.31     | 0.18                | 0.22       |
| (1,1504) | 1:147:A:ILE:HD12 | 1:157:A:VAL:HG13 | 4                   | 0.31     | 0.18                | 0.22       |
| (1,1504) | 1:147:A:ILE:HD11 | 1:157:A:VAL:HG21 | 4                   | 0.31     | 0.18                | 0.22       |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD21 | 4                   | 0.28     | 0.11                | 0.28       |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD22 | 4                   | 0.28     | 0.11                | 0.28       |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD23 | 4                   | 0.28     | 0.11                | 0.28       |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD11 | 4                   | 0.28     | 0.11                | 0.28       |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD12 | 4                   | 0.28     | 0.11                | 0.28       |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD13 | 4                   | 0.28     | 0.11                | 0.28       |
| (1,2013) | 1:98:A:GLU:HG2   | 1:98:A:GLU:H     | 4                   | 0.27     | 0.11                | 0.26       |
| (1,2826) | 1:143:A:TRP:HZ2  | 1:147:A:ILE:HD12 | 4                   | 0.26     | 0.16                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2826) | 1:143:A:TRP:HZ2  | 1:147:A:ILE:HD11 | 4                   | 0.26     | 0.16                | 0.2        |
| (1,1470) | 1:159:A:PRO:HD3  | 1:162:A:LYS:HG3  | 4                   | 0.24     | 0.08                | 0.26       |
| (1,149)  | 1:135:A:ASP:H    | 1:133:A:GLU:HG2  | 4                   | 0.22     | 0.09                | 0.18       |
| (1,149)  | 1:135:A:ASP:H    | 1:133:A:GLU:HG3  | 4                   | 0.22     | 0.09                | 0.18       |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG21 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG22 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG23 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,1793) | 1:144:A:LYS:HD3  | 1:147:A:ILE:HG21 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,1793) | 1:144:A:LYS:HD3  | 1:147:A:ILE:HG22 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,1793) | 1:144:A:LYS:HD3  | 1:147:A:ILE:HG23 | 4                   | 0.22     | 0.1                 | 0.2        |
| (1,1616) | 1:66:A:VAL:HG11  | 1:131:A:VAL:HB   | 4                   | 0.2      | 0.08                | 0.18       |
| (1,1616) | 1:66:A:VAL:HG12  | 1:131:A:VAL:HB   | 4                   | 0.2      | 0.08                | 0.18       |
| (1,1616) | 1:66:A:VAL:HG13  | 1:131:A:VAL:HB   | 4                   | 0.2      | 0.08                | 0.18       |
| (1,1616) | 1:66:A:VAL:HG21  | 1:131:A:VAL:HB   | 4                   | 0.2      | 0.08                | 0.18       |
| (1,1616) | 1:66:A:VAL:HG22  | 1:131:A:VAL:HB   | 4                   | 0.2      | 0.08                | 0.18       |
| (1,1616) | 1:66:A:VAL:HG23  | 1:131:A:VAL:HB   | 4                   | 0.2      | 0.08                | 0.18       |
| (1,1552) | 1:111:A:SER:HA   | 1:114:A:ALA:H    | 4                   | 0.19     | 0.04                | 0.2        |
| (1,1618) | 1:121:A:GLU:HG3  | 1:94:A:ASP:HB3   | 4                   | 0.19     | 0.04                | 0.18       |
| (1,1618) | 1:121:A:GLU:HG2  | 1:94:A:ASP:HB3   | 4                   | 0.19     | 0.04                | 0.18       |
| (1,275)  | 1:150:A:HIS:H    | 1:149:A:GLU:HB2  | 4                   | 0.18     | 0.04                | 0.18       |
| (1,275)  | 1:150:A:HIS:H    | 1:149:A:GLU:HB3  | 4                   | 0.18     | 0.04                | 0.18       |
| (1,1548) | 1:104:A:ILE:HD11 | 1:144:A:LYS:H    | 4                   | 0.16     | 0.02                | 0.16       |
| (1,1548) | 1:104:A:ILE:HD13 | 1:144:A:LYS:H    | 4                   | 0.16     | 0.02                | 0.16       |
| (1,1548) | 1:104:A:ILE:HD12 | 1:144:A:LYS:H    | 4                   | 0.16     | 0.02                | 0.16       |
| (1,150)  | 1:142:A:ALA:H    | 1:145:A:LEU:HB2  | 4                   | 0.13     | 0.03                | 0.11       |
| (1,1831) | 1:125:A:SER:HB2  | 1:74:A:LEU:HB3   | 3                   | 0.79     | 0.06                | 0.82       |
| (1,1455) | 1:170:A:LYS:HG3  | 1:169:A:VAL:HA   | 3                   | 0.56     | 0.22                | 0.61       |
| (1,1455) | 1:170:A:LYS:HG3  | 1:171:A:VAL:HA   | 3                   | 0.56     | 0.22                | 0.61       |
| (1,1455) | 1:170:A:LYS:HG2  | 1:171:A:VAL:HA   | 3                   | 0.56     | 0.22                | 0.61       |
| (1,71)   | 1:71:A:GLU:H     | 1:69:A:LEU:HG    | 3                   | 0.55     | 0.11                | 0.61       |
| (1,1577) | 1:150:A:HIS:HB3  | 1:154:A:THR:HG22 | 3                   | 0.55     | 0.14                | 0.64       |
| (1,1476) | 1:66:A:VAL:HG21  | 1:71:A:GLU:HG3   | 3                   | 0.54     | 0.27                | 0.72       |
| (1,1476) | 1:66:A:VAL:HG22  | 1:71:A:GLU:HG3   | 3                   | 0.54     | 0.27                | 0.72       |
| (1,1476) | 1:66:A:VAL:HG23  | 1:71:A:GLU:HG3   | 3                   | 0.54     | 0.27                | 0.72       |
| (1,1476) | 1:66:A:VAL:HG11  | 1:71:A:GLU:HG3   | 3                   | 0.54     | 0.27                | 0.72       |
| (1,1476) | 1:66:A:VAL:HG12  | 1:71:A:GLU:HG3   | 3                   | 0.54     | 0.27                | 0.72       |
| (1,1476) | 1:66:A:VAL:HG13  | 1:71:A:GLU:HG3   | 3                   | 0.54     | 0.27                | 0.72       |
| (1,1391) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE2  | 3                   | 0.41     | 0.2                 | 0.35       |
| (1,1391) | 1:162:A:LYS:HB3  | 1:162:A:LYS:HE3  | 3                   | 0.41     | 0.2                 | 0.35       |
| (1,1391) | 1:162:A:LYS:HB2  | 1:162:A:LYS:HE2  | 3                   | 0.41     | 0.2                 | 0.35       |
| (1,1500) | 1:151:A:ILE:HG23 | 1:152:A:LYS:HE2  | 3                   | 0.4      | 0.17                | 0.46       |
| (1,1500) | 1:151:A:ILE:HG21 | 1:152:A:LYS:HE3  | 3                   | 0.4      | 0.17                | 0.46       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1500) | 1:151:A:ILE:HG23 | 1:150:A:HIS:HB2  | 3                   | 0.4      | 0.17                | 0.46       |
| (1,1612) | 1:148:A:GLU:HG2  | 1:152:A:LYS:HE2  | 3                   | 0.39     | 0.18                | 0.32       |
| (1,2869) | 1:115:A:HIS:HE1  | 1:116:A:LEU:HD21 | 3                   | 0.34     | 0.15                | 0.41       |
| (1,2869) | 1:115:A:HIS:HE1  | 1:112:A:VAL:HG13 | 3                   | 0.34     | 0.15                | 0.41       |
| (1,2869) | 1:115:A:HIS:HE1  | 1:112:A:VAL:HG11 | 3                   | 0.34     | 0.15                | 0.41       |
| (1,31)   | 1:87:A:SER:H     | 1:134:A:PRO:HB3  | 3                   | 0.32     | 0.02                | 0.32       |
| (1,31)   | 1:87:A:SER:H     | 1:106:A:ARG:HB3  | 3                   | 0.32     | 0.02                | 0.32       |
| (1,26)   | 1:125:A:SER:H    | 1:95:A:LYS:HD2   | 3                   | 0.3      | 0.03                | 0.28       |
| (1,26)   | 1:125:A:SER:H    | 1:92:A:VAL:HB    | 3                   | 0.3      | 0.03                | 0.28       |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD11 | 3                   | 0.3      | 0.09                | 0.31       |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD12 | 3                   | 0.3      | 0.09                | 0.31       |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD13 | 3                   | 0.3      | 0.09                | 0.31       |
| (1,347)  | 1:70:A:THR:H     | 1:69:A:LEU:HB2   | 3                   | 0.28     | 0.05                | 0.3        |
| (1,1376) | 1:162:A:LYS:HD2  | 1:157:A:VAL:HG13 | 3                   | 0.27     | 0.17                | 0.16       |
| (1,1376) | 1:162:A:LYS:HD2  | 1:157:A:VAL:HG11 | 3                   | 0.27     | 0.17                | 0.16       |
| (1,1376) | 1:162:A:LYS:HD2  | 1:157:A:VAL:HG23 | 3                   | 0.27     | 0.17                | 0.16       |
| (1,396)  | 1:100:A:GLN:H    | 1:98:A:GLU:HB3   | 3                   | 0.24     | 0.09                | 0.26       |
| (1,396)  | 1:100:A:GLN:H    | 1:98:A:GLU:HB2   | 3                   | 0.24     | 0.09                | 0.26       |
| (1,295)  | 1:108:A:ILE:H    | 1:87:A:SER:HB2   | 3                   | 0.22     | 0.08                | 0.25       |
| (1,295)  | 1:108:A:ILE:H    | 1:87:A:SER:HB3   | 3                   | 0.22     | 0.08                | 0.25       |
| (1,1586) | 1:95:A:LYS:HD3   | 1:95:A:LYS:H     | 3                   | 0.19     | 0.05                | 0.21       |
| (1,1586) | 1:95:A:LYS:HD2   | 1:95:A:LYS:H     | 3                   | 0.19     | 0.05                | 0.21       |
| (1,95)   | 1:153:A:VAL:H    | 1:152:A:LYS:HB2  | 3                   | 0.17     | 0.04                | 0.2        |
| (1,95)   | 1:153:A:VAL:H    | 1:153:A:VAL:HB   | 3                   | 0.17     | 0.04                | 0.2        |
| (1,1834) | 1:147:A:ILE:HD12 | 1:143:A:TRP:HZ2  | 3                   | 0.17     | 0.06                | 0.14       |
| (1,1834) | 1:147:A:ILE:HD11 | 1:143:A:TRP:HZ2  | 3                   | 0.17     | 0.06                | 0.14       |
| (1,190)  | 1:151:A:ILE:H    | 1:147:A:ILE:HG21 | 3                   | 0.16     | 0.04                | 0.13       |
| (1,190)  | 1:151:A:ILE:H    | 1:147:A:ILE:HG22 | 3                   | 0.16     | 0.04                | 0.13       |
| (1,1724) | 1:122:A:LEU:HD13 | 1:101:A:PHE:H    | 3                   | 0.13     | 0.03                | 0.11       |
| (1,1724) | 1:122:A:LEU:HD11 | 1:101:A:PHE:H    | 3                   | 0.13     | 0.03                | 0.11       |
| (1,1897) | 1:85:A:SER:HB2   | 1:84:A:PRO:HA    | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,1751) | 1:108:A:ILE:HG21 | 1:111:A:SER:H    | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1751) | 1:108:A:ILE:HG23 | 1:111:A:SER:H    | 3                   | 0.12     | 0.02                | 0.11       |
| (1,881)  | 1:127:A:LYS:H    | 1:93:A:TYR:HD1   | 2                   | 3.36     | 0.21                | 3.36       |
| (1,2921) | 1:93:A:TYR:HE1   | 1:127:A:LYS:HB2  | 2                   | 2.54     | 0.23                | 2.54       |
| (1,2646) | 1:91:A:ALA:HB1   | 1:93:A:TYR:HD1   | 2                   | 1.66     | 0.13                | 1.66       |
| (1,2646) | 1:91:A:ALA:HB2   | 1:93:A:TYR:HD1   | 2                   | 1.66     | 0.13                | 1.66       |
| (1,2646) | 1:91:A:ALA:HB3   | 1:93:A:TYR:HD1   | 2                   | 1.66     | 0.13                | 1.66       |
| (1,882)  | 1:127:A:LYS:H    | 1:93:A:TYR:HE1   | 2                   | 1.6      | 0.26                | 1.6        |
| (1,1006) | 1:93:A:TYR:H     | 1:93:A:TYR:HD1   | 2                   | 1.24     | 0.0                 | 1.24       |
| (1,1000) | 1:93:A:TYR:H     | 1:93:A:TYR:HE1   | 2                   | 0.92     | 0.0                 | 0.92       |
| (1,2847) | 1:93:A:TYR:HE1   | 1:93:A:TYR:H     | 2                   | 0.92     | 0.0                 | 0.92       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,535)  | 1:125:A:SER:H    | 1:93:A:TYR:HD1   | 2                   | 0.6      | 0.08                | 0.6        |
| (1,1543) | 1:119:A:VAL:HG11 | 1:168:A:PHE:HB3  | 2                   | 0.6      | 0.42                | 0.6        |
| (1,1543) | 1:119:A:VAL:HG13 | 1:168:A:PHE:HB3  | 2                   | 0.6      | 0.42                | 0.6        |
| (1,1435) | 1:84:A:PRO:HG3   | 1:130:A:ILE:HD13 | 2                   | 0.56     | 0.38                | 0.56       |
| (1,1435) | 1:84:A:PRO:HG3   | 1:130:A:ILE:HD12 | 2                   | 0.56     | 0.38                | 0.56       |
| (1,1859) | 1:77:A:ILE:HD13  | 1:76:A:PRO:HB2   | 2                   | 0.55     | 0.15                | 0.55       |
| (1,1859) | 1:77:A:ILE:HD11  | 1:76:A:PRO:HB2   | 2                   | 0.55     | 0.15                | 0.55       |
| (1,1963) | 1:154:A:THR:HB   | 1:156:A:LYS:HE2  | 2                   | 0.49     | 0.09                | 0.49       |
| (1,1963) | 1:154:A:THR:HB   | 1:156:A:LYS:HE3  | 2                   | 0.49     | 0.09                | 0.49       |
| (1,346)  | 1:155:A:GLY:H    | 1:156:A:LYS:HG3  | 2                   | 0.46     | 0.17                | 0.46       |
| (1,346)  | 1:155:A:GLY:H    | 1:156:A:LYS:HG2  | 2                   | 0.46     | 0.17                | 0.46       |
| (1,1666) | 1:156:A:LYS:HG3  | 1:155:A:GLY:H    | 2                   | 0.46     | 0.17                | 0.46       |
| (1,1666) | 1:156:A:LYS:HG2  | 1:155:A:GLY:H    | 2                   | 0.46     | 0.17                | 0.46       |
| (1,202)  | 1:156:A:LYS:H    | 1:156:A:LYS:HG3  | 2                   | 0.46     | 0.08                | 0.46       |
| (1,324)  | 1:154:A:THR:H    | 1:156:A:LYS:HG2  | 2                   | 0.44     | 0.01                | 0.44       |
| (1,1432) | 1:95:A:LYS:HD3   | 1:123:A:CYS:H    | 2                   | 0.42     | 0.1                 | 0.42       |
| (1,111)  | 1:148:A:GLU:H    | 1:148:A:GLU:HG3  | 2                   | 0.4      | 0.07                | 0.4        |
| (1,1826) | 1:167:A:THR:HA   | 1:170:A:LYS:HB3  | 2                   | 0.38     | 0.24                | 0.38       |
| (1,263)  | 1:146:A:TRP:HE1  | 1:68:A:SER:HB3   | 2                   | 0.34     | 0.2                 | 0.34       |
| (1,2791) | 1:90:A:TYR:HE1   | 1:112:A:VAL:HG22 | 2                   | 0.34     | 0.08                | 0.34       |
| (1,1385) | 1:170:A:LYS:HG3  | 1:170:A:LYS:HE2  | 2                   | 0.3      | 0.02                | 0.3        |
| (1,1385) | 1:170:A:LYS:HG2  | 1:170:A:LYS:HE3  | 2                   | 0.3      | 0.02                | 0.3        |
| (1,1393) | 1:170:A:LYS:HE2  | 1:170:A:LYS:HG3  | 2                   | 0.3      | 0.02                | 0.3        |
| (1,1393) | 1:170:A:LYS:HE3  | 1:170:A:LYS:HG2  | 2                   | 0.3      | 0.02                | 0.3        |
| (1,280)  | 1:67:A:LYS:H     | 1:67:A:LYS:HG3   | 2                   | 0.3      | 0.03                | 0.3        |
| (1,205)  | 1:153:A:VAL:H    | 1:152:A:LYS:HD2  | 2                   | 0.26     | 0.08                | 0.26       |
| (1,352)  | 1:124:A:GLY:H    | 1:95:A:LYS:HD3   | 2                   | 0.26     | 0.1                 | 0.26       |
| (1,352)  | 1:124:A:GLY:H    | 1:95:A:LYS:HD2   | 2                   | 0.26     | 0.1                 | 0.26       |
| (1,1584) | 1:95:A:LYS:HD3   | 1:124:A:GLY:H    | 2                   | 0.26     | 0.1                 | 0.26       |
| (1,1584) | 1:95:A:LYS:HD2   | 1:124:A:GLY:H    | 2                   | 0.26     | 0.1                 | 0.26       |
| (1,305)  | 1:146:A:TRP:HE1  | 1:145:A:LEU:HD21 | 2                   | 0.25     | 0.08                | 0.25       |
| (1,305)  | 1:146:A:TRP:HE1  | 1:145:A:LEU:HD22 | 2                   | 0.25     | 0.08                | 0.25       |
| (1,305)  | 1:146:A:TRP:HE1  | 1:145:A:LEU:HD23 | 2                   | 0.25     | 0.08                | 0.25       |
| (1,1537) | 1:154:A:THR:HB   | 1:156:A:LYS:HB3  | 2                   | 0.25     | 0.09                | 0.25       |
| (1,343)  | 1:96:A:SER:H     | 1:95:A:LYS:HD2   | 2                   | 0.24     | 0.14                | 0.24       |
| (1,343)  | 1:96:A:SER:H     | 1:95:A:LYS:HD3   | 2                   | 0.24     | 0.14                | 0.24       |
| (1,345)  | 1:124:A:GLY:H    | 1:77:A:ILE:HG12  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,356)  | 1:100:A:GLN:H    | 1:102:A:VAL:HG12 | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,356)  | 1:100:A:GLN:H    | 1:102:A:VAL:HG11 | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,1578) | 1:77:A:ILE:HG12  | 1:124:A:GLY:H    | 2                   | 0.22     | 0.01                | 0.22       |
| (1,1753) | 1:106:A:ARG:HG3  | 1:87:A:SER:HB2   | 2                   | 0.21     | 0.04                | 0.21       |
| (1,410)  | 1:95:A:LYS:H     | 1:95:A:LYS:HE3   | 2                   | 0.21     | 0.09                | 0.21       |

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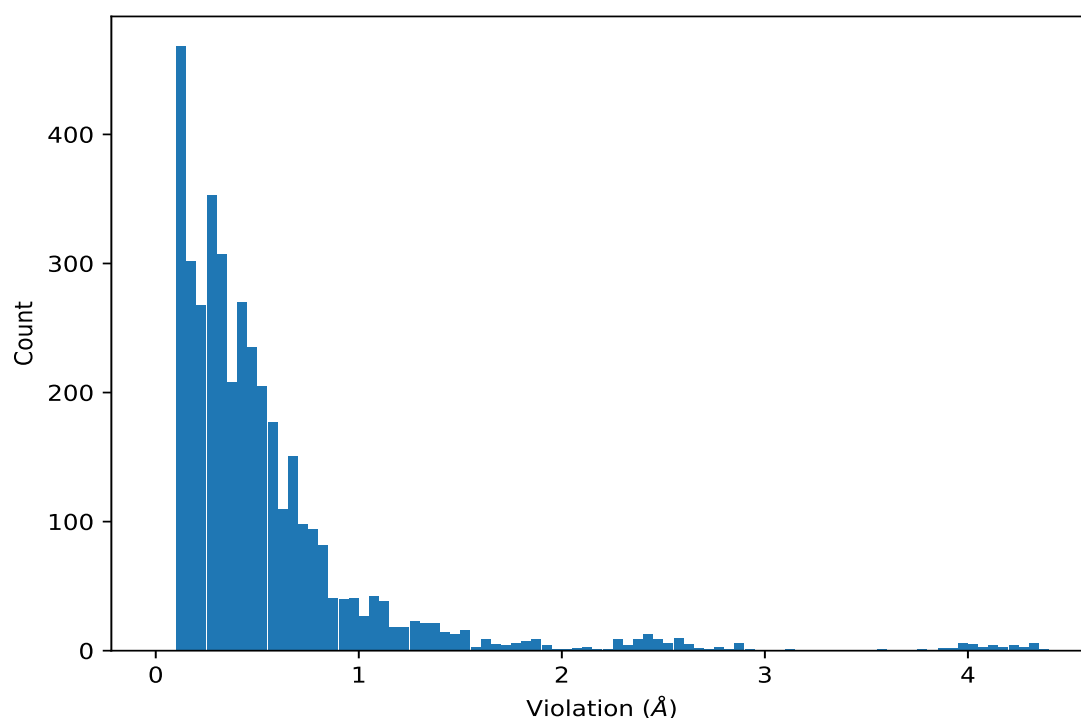
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1863) | 1:95:A:LYS:HE3   | 1:95:A:LYS:H     | 2                   | 0.21     | 0.09                | 0.21       |
| (1,2027) | 1:70:A:THR:HB    | 1:149:A:GLU:HB3  | 2                   | 0.21     | 0.09                | 0.21       |
| (1,1450) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HB2   | 2                   | 0.2      | 0.03                | 0.2        |
| (1,1803) | 1:152:A:LYS:HD2  | 1:152:A:LYS:HE3  | 2                   | 0.2      | 0.01                | 0.2        |
| (1,1829) | 1:84:A:PRO:HD3   | 1:83:A:ILE:HG22  | 2                   | 0.2      | 0.05                | 0.2        |
| (1,1969) | 1:152:A:LYS:HE3  | 1:152:A:LYS:HD2  | 2                   | 0.2      | 0.01                | 0.2        |
| (1,237)  | 1:92:A:VAL:H     | 1:90:A:TYR:HB2   | 2                   | 0.17     | 0.0                 | 0.17       |
| (1,244)  | 1:123:A:CYS:H    | 1:95:A:LYS:H     | 2                   | 0.16     | 0.02                | 0.16       |
| (1,1761) | 1:170:A:LYS:HD2  | 1:170:A:LYS:H    | 2                   | 0.16     | 0.04                | 0.16       |
| (1,4)    | 1:142:A:ALA:H    | 1:145:A:LEU:HB2  | 2                   | 0.15     | 0.04                | 0.15       |
| (1,80)   | 1:144:A:LYS:H    | 1:143:A:TRP:HB2  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,1555) | 1:148:A:GLU:HG3  | 1:147:A:ILE:HG21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1640) | 1:159:A:PRO:HB3  | 1:162:A:LYS:HE2  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,1640) | 1:159:A:PRO:HB3  | 1:162:A:LYS:HE3  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,1710) | 1:156:A:LYS:HG3  | 1:100:A:GLN:HA   | 2                   | 0.13     | 0.03                | 0.13       |
| (1,1710) | 1:156:A:LYS:HG2  | 1:100:A:GLN:HA   | 2                   | 0.13     | 0.03                | 0.13       |
| (1,1904) | 1:100:A:GLN:HA   | 1:156:A:LYS:HG3  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,1904) | 1:100:A:GLN:HA   | 1:156:A:LYS:HG2  | 2                   | 0.13     | 0.03                | 0.13       |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG11 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG13 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1042) | 1:100:A:GLN:H    | 1:150:A:HIS:HB3  | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,948)  | 1:102:A:VAL:H    | 1:160:A:GLY:HA3  | 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) |
|---------|---------------|----------------|----------|---------------|
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 5        | 4.37          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 9        | 4.34          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 10       | 4.34          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 15       | 4.34          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 17       | 4.34          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 2        | 4.3           |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 18       | 4.3           |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 11       | 4.28          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 13       | 4.27          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 20       | 4.26          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 14       | 4.24          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 16       | 4.23          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 6        | 4.22          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HD1 | 8        | 4.22          |
| (1,648) | 1:88:A:GLY:H  | 1:90:A:TYR:HD1 | 19       | 4.15          |
| (1,232) | 1:105:A:SER:H | 1:90:A:TYR:HE1 | 7        | 4.15          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,232)  | 1:105:A:SER:H    | 1:90:A:TYR:HE1  | 12       | 4.15          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 3        | 4.14          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 9        | 4.12          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 13       | 4.11          |
| (1,232)  | 1:105:A:SER:H    | 1:90:A:TYR:HE1  | 3        | 4.11          |
| (1,232)  | 1:105:A:SER:H    | 1:90:A:TYR:HD1  | 1        | 4.1           |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 6        | 4.07          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 11       | 4.05          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 5        | 4.04          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 10       | 4.04          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 8        | 4.03          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 16       | 4.01          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 17       | 4.0           |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 1        | 3.98          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 20       | 3.98          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 2        | 3.97          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 15       | 3.97          |
| (1,232)  | 1:105:A:SER:H    | 1:90:A:TYR:HD1  | 19       | 3.97          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 12       | 3.96          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 7        | 3.92          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 14       | 3.92          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 4        | 3.9           |
| (1,232)  | 1:105:A:SER:H    | 1:90:A:TYR:HE1  | 4        | 3.87          |
| (1,648)  | 1:88:A:GLY:H     | 1:90:A:TYR:HD1  | 18       | 3.79          |
| (1,881)  | 1:127:A:LYS:H    | 1:93:A:TYR:HD1  | 19       | 3.57          |
| (1,881)  | 1:127:A:LYS:H    | 1:93:A:TYR:HD1  | 6        | 3.15          |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1  | 6        | 2.91          |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1  | 9        | 2.89          |
| (1,1769) | 1:104:A:ILE:HG23 | 1:90:A:TYR:HD1  | 19       | 2.88          |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1  | 15       | 2.87          |
| (1,1769) | 1:104:A:ILE:HG23 | 1:90:A:TYR:HD1  | 10       | 2.86          |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1  | 16       | 2.86          |
| (1,1769) | 1:104:A:ILE:HG21 | 1:90:A:TYR:HD1  | 1        | 2.85          |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1  | 2        | 2.83          |
| (1,1769) | 1:104:A:ILE:HG21 | 1:90:A:TYR:HD1  | 5        | 2.79          |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1  | 18       | 2.78          |
| (1,2921) | 1:93:A:TYR:HE1   | 1:127:A:LYS:HB2 | 19       | 2.77          |
| (1,1769) | 1:104:A:ILE:HG21 | 1:90:A:TYR:HD1  | 14       | 2.71          |
| (1,1769) | 1:104:A:ILE:HG21 | 1:90:A:TYR:HD1  | 17       | 2.67          |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1  | 8        | 2.66          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1  | 4        | 2.64          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 4        | 2.64          |

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| Key      | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|----------|------------------|----------------|----------|---------------|
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 4        | 2.64          |
| (1,1769) | 1:104:A:ILE:HG21 | 1:90:A:TYR:HD1 | 12       | 2.61          |
| (1,1769) | 1:104:A:ILE:HG21 | 1:90:A:TYR:HD1 | 11       | 2.6           |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 12       | 2.59          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 12       | 2.59          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 12       | 2.59          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 3        | 2.56          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 3        | 2.56          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 3        | 2.56          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 8        | 2.56          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 8        | 2.56          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 8        | 2.56          |
| (1,1769) | 1:104:A:ILE:HG22 | 1:90:A:TYR:HD1 | 20       | 2.56          |
| (1,1769) | 1:104:A:ILE:HG23 | 1:90:A:TYR:HD1 | 7        | 2.55          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 14       | 2.54          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 14       | 2.54          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 14       | 2.54          |
| (1,1769) | 1:104:A:ILE:HG23 | 1:90:A:TYR:HD1 | 3        | 2.53          |
| (1,1769) | 1:104:A:ILE:HG23 | 1:90:A:TYR:HD1 | 4        | 2.51          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 17       | 2.47          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 17       | 2.47          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 17       | 2.47          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 7        | 2.46          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 7        | 2.46          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 7        | 2.46          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 20       | 2.45          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 20       | 2.45          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 20       | 2.45          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 19       | 2.43          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 19       | 2.43          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 19       | 2.43          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 11       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 11       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 11       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 13       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 13       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 13       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 15       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1 | 15       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1 | 15       | 2.42          |
| (1,1769) | 1:104:A:ILE:HG21 | 1:90:A:TYR:HD1 | 13       | 2.42          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1 | 16       | 2.38          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 16       | 2.38          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1  | 16       | 2.38          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1  | 18       | 2.38          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 18       | 2.38          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1  | 18       | 2.38          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1  | 9        | 2.35          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 9        | 2.35          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1  | 9        | 2.35          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1  | 2        | 2.33          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 2        | 2.33          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1  | 2        | 2.33          |
| (1,2921) | 1:93:A:TYR:HE1   | 1:127:A:LYS:HB2 | 6        | 2.32          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1  | 1        | 2.29          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 1        | 2.29          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1  | 1        | 2.29          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1  | 10       | 2.29          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 10       | 2.29          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1  | 10       | 2.29          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1  | 5        | 2.28          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 5        | 2.28          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1  | 5        | 2.28          |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H   | 5        | 2.21          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2  | 16       | 2.15          |
| (1,2202) | 1:108:A:ILE:HD11 | 1:90:A:TYR:HD1  | 6        | 2.11          |
| (1,2202) | 1:108:A:ILE:HD12 | 1:90:A:TYR:HD1  | 6        | 2.11          |
| (1,2202) | 1:108:A:ILE:HD13 | 1:90:A:TYR:HD1  | 6        | 2.11          |
| (1,1419) | 1:92:A:VAL:HG13  | 1:101:A:PHE:H   | 10       | 2.09          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 19       | 2.09          |
| (1,1438) | 1:104:A:ILE:HD12 | 1:90:A:TYR:HE2  | 14       | 2.02          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 7        | 1.97          |
| (1,1438) | 1:104:A:ILE:HD11 | 1:90:A:TYR:HE2  | 18       | 1.94          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 4        | 1.92          |
| (1,1419) | 1:92:A:VAL:HG23  | 1:101:A:PHE:H   | 9        | 1.91          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 3        | 1.91          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2  | 4        | 1.9           |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 11       | 1.89          |
| (1,1438) | 1:104:A:ILE:HD11 | 1:90:A:TYR:HE2  | 6        | 1.87          |
| (1,1438) | 1:104:A:ILE:HD11 | 1:90:A:TYR:HE2  | 7        | 1.87          |
| (1,1419) | 1:92:A:VAL:HG13  | 1:101:A:PHE:H   | 8        | 1.87          |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H   | 13       | 1.87          |
| (1,882)  | 1:127:A:LYS:H    | 1:93:A:TYR:HE1  | 19       | 1.86          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2  | 19       | 1.85          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1419) | 1:92:A:VAL:HG22  | 1:101:A:PHE:H   | 18       | 1.85          |
| (1,1438) | 1:104:A:ILE:HD12 | 1:90:A:TYR:HE2  | 3        | 1.84          |
| (1,1419) | 1:92:A:VAL:HG21  | 1:101:A:PHE:H   | 16       | 1.83          |
| (1,1419) | 1:92:A:VAL:HG13  | 1:101:A:PHE:H   | 20       | 1.83          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 13       | 1.83          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 20       | 1.83          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2  | 13       | 1.82          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 14       | 1.8           |
| (1,2646) | 1:91:A:ALA:HB1   | 1:93:A:TYR:HD1  | 19       | 1.79          |
| (1,2646) | 1:91:A:ALA:HB2   | 1:93:A:TYR:HD1  | 19       | 1.79          |
| (1,2646) | 1:91:A:ALA:HB3   | 1:93:A:TYR:HD1  | 19       | 1.79          |
| (1,1438) | 1:104:A:ILE:HD12 | 1:90:A:TYR:HE2  | 12       | 1.79          |
| (1,1419) | 1:92:A:VAL:HG13  | 1:101:A:PHE:H   | 4        | 1.78          |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H   | 19       | 1.76          |
| (1,1419) | 1:92:A:VAL:HG12  | 1:101:A:PHE:H   | 1        | 1.73          |
| (1,1419) | 1:92:A:VAL:HG13  | 1:101:A:PHE:H   | 7        | 1.73          |
| (1,1438) | 1:104:A:ILE:HD11 | 1:90:A:TYR:HE2  | 1        | 1.72          |
| (1,1454) | 1:89:A:VAL:HG21  | 1:139:A:LEU:HB2 | 8        | 1.71          |
| (1,1557) | 1:147:A:ILE:HD12 | 1:144:A:LYS:HE2 | 13       | 1.7           |
| (1,1454) | 1:89:A:VAL:HG13  | 1:139:A:LEU:HG  | 16       | 1.68          |
| (1,1438) | 1:104:A:ILE:HD12 | 1:90:A:TYR:HE2  | 10       | 1.67          |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H   | 3        | 1.66          |
| (1,1419) | 1:92:A:VAL:HG13  | 1:101:A:PHE:H   | 12       | 1.66          |
| (1,1454) | 1:89:A:VAL:HG22  | 1:139:A:LEU:HB2 | 14       | 1.63          |
| (1,1438) | 1:104:A:ILE:HD11 | 1:90:A:TYR:HE2  | 8        | 1.63          |
| (1,1419) | 1:92:A:VAL:HG12  | 1:101:A:PHE:H   | 2        | 1.63          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 2        | 1.63          |
| (1,1984) | 1:69:A:LEU:HD11  | 1:68:A:SER:H    | 4        | 1.62          |
| (1,1454) | 1:89:A:VAL:HG11  | 1:139:A:LEU:HG  | 17       | 1.62          |
| (1,1514) | 1:147:A:ILE:HD13 | 1:157:A:VAL:H   | 2        | 1.61          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2  | 17       | 1.61          |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H   | 15       | 1.6           |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 15       | 1.58          |
| (1,1676) | 1:99:A:LEU:HD21  | 1:126:A:VAL:HB  | 9        | 1.57          |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H   | 14       | 1.56          |
| (1,1557) | 1:147:A:ILE:HD11 | 1:143:A:TRP:HB2 | 5        | 1.54          |
| (1,2646) | 1:91:A:ALA:HB1   | 1:93:A:TYR:HD1  | 6        | 1.53          |
| (1,2646) | 1:91:A:ALA:HB2   | 1:93:A:TYR:HD1  | 6        | 1.53          |
| (1,2646) | 1:91:A:ALA:HB3   | 1:93:A:TYR:HD1  | 6        | 1.53          |
| (1,1454) | 1:89:A:VAL:HG22  | 1:139:A:LEU:HB2 | 12       | 1.53          |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H   | 17       | 1.53          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1 | 5        | 1.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1438) | 1:104:A:ILE:HD12 | 1:90:A:TYR:HE2   | 2        | 1.52          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2   | 5        | 1.52          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2   | 20       | 1.52          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 3        | 1.51          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 2        | 1.5           |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 7        | 1.5           |
| (1,1514) | 1:147:A:ILE:HD11 | 1:157:A:VAL:H    | 14       | 1.5           |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG11  | 3        | 1.5           |
| (1,1419) | 1:92:A:VAL:HG12  | 1:101:A:PHE:H    | 11       | 1.5           |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 9        | 1.49          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 10       | 1.49          |
| (1,1557) | 1:147:A:ILE:HD11 | 1:144:A:LYS:HE3  | 3        | 1.49          |
| (1,1454) | 1:89:A:VAL:HG11  | 1:139:A:LEU:HG   | 4        | 1.49          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2   | 9        | 1.49          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 8        | 1.48          |
| (1,2011) | 1:151:A:ILE:HD13 | 1:157:A:VAL:H    | 8        | 1.47          |
| (1,1557) | 1:147:A:ILE:HD11 | 1:144:A:LYS:HE2  | 10       | 1.47          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD21 | 5        | 1.47          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD13 | 20       | 1.47          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 16       | 1.47          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 16       | 1.46          |
| (1,1454) | 1:89:A:VAL:HG21  | 1:139:A:LEU:HB2  | 6        | 1.46          |
| (1,1722) | 1:69:A:LEU:HD22  | 1:150:A:HIS:HE1  | 1        | 1.45          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 18       | 1.45          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 6        | 1.44          |
| (1,1438) | 1:104:A:ILE:HD13 | 1:90:A:TYR:HE2   | 11       | 1.44          |
| (1,1400) | 1:99:A:LEU:HD11  | 1:98:A:GLU:HB3   | 6        | 1.44          |
| (1,1557) | 1:147:A:ILE:HD12 | 1:143:A:TRP:HB2  | 7        | 1.43          |
| (1,1557) | 1:147:A:ILE:HD11 | 1:143:A:TRP:HB2  | 19       | 1.43          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 12       | 1.42          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 19       | 1.42          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 20       | 1.42          |
| (1,1722) | 1:69:A:LEU:HD22  | 1:150:A:HIS:HE1  | 11       | 1.42          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1  | 9        | 1.42          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD11 | 12       | 1.41          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 19       | 1.41          |
| (1,2011) | 1:151:A:ILE:HD11 | 1:157:A:VAL:H    | 1        | 1.39          |
| (1,1438) | 1:104:A:ILE:HD12 | 1:90:A:TYR:HE2   | 15       | 1.39          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 7        | 1.39          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 16       | 1.39          |
| (1,1519) | 1:66:A:VAL:HG12  | 1:89:A:VAL:HG21  | 13       | 1.38          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1  | 12       | 1.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 10       | 1.38          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 5        | 1.37          |
| (1,1557) | 1:147:A:ILE:HD12 | 1:143:A:TRP:HB2  | 9        | 1.37          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG22  | 4        | 1.37          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG13 | 4        | 1.37          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 6        | 1.37          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 12       | 1.37          |
| (1,1454) | 1:89:A:VAL:HG13  | 1:139:A:LEU:HG   | 3        | 1.36          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG22  | 12       | 1.36          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 3        | 1.36          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 5        | 1.36          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 14       | 1.36          |
| (1,882)  | 1:127:A:LYS:H    | 1:93:A:TYR:HE1   | 6        | 1.35          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 8        | 1.35          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 20       | 1.35          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 18       | 1.34          |
| (1,1722) | 1:69:A:LEU:HD21  | 1:149:A:GLU:H    | 15       | 1.34          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 13       | 1.34          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG13 | 16       | 1.33          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 4        | 1.32          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 11       | 1.32          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 13       | 1.32          |
| (1,1433) | 1:136:A:LYS:HD2  | 1:104:A:ILE:HG23 | 1        | 1.32          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 15       | 1.32          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 19       | 1.32          |
| (1,1516) | 1:116:A:LEU:HD21 | 1:168:A:PHE:HD1  | 10       | 1.31          |
| (1,1514) | 1:147:A:ILE:HD11 | 1:157:A:VAL:H    | 16       | 1.31          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:116:A:LEU:HD23 | 18       | 1.31          |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD13 | 8        | 1.31          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 17       | 1.31          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 14       | 1.3           |
| (1,1433) | 1:117:A:LYS:HD3  | 1:116:A:LEU:HD23 | 13       | 1.3           |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG21  | 17       | 1.3           |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 2        | 1.3           |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 18       | 1.3           |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE2   | 5        | 1.3           |
| (1,1679) | 1:74:A:LEU:HD21  | 1:76:A:PRO:HG3   | 12       | 1.29          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD11 | 2        | 1.29          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD11 | 13       | 1.29          |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG12  | 12       | 1.29          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 6        | 1.29          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 11       | 1.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG12 | 15       | 1.29          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 17       | 1.28          |
| (1,1557) | 1:147:A:ILE:HD13 | 1:144:A:LYS:HE2  | 20       | 1.28          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG21 | 15       | 1.28          |
| (1,1419) | 1:92:A:VAL:HG11  | 1:101:A:PHE:H    | 6        | 1.28          |
| (1,1377) | 1:89:A:VAL:HG11  | 1:66:A:VAL:HG11  | 14       | 1.28          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG11 | 1        | 1.28          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG13 | 9        | 1.28          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 6        | 1.28          |
| (1,1722) | 1:69:A:LEU:HD23  | 1:149:A:GLU:H    | 12       | 1.27          |
| (1,1514) | 1:147:A:ILE:HD12 | 1:157:A:VAL:H    | 11       | 1.27          |
| (1,1377) | 1:89:A:VAL:HG11  | 1:66:A:VAL:HG13  | 17       | 1.27          |
| (1,29)   | 1:108:A:ILE:H    | 1:128:A:VAL:HG13 | 19       | 1.27          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 4        | 1.26          |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD13 | 7        | 1.26          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 10       | 1.26          |
| (1,1454) | 1:89:A:VAL:HG13  | 1:139:A:LEU:HG   | 7        | 1.25          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 15       | 1.24          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 11       | 1.24          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 15       | 1.24          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG22 | 8        | 1.24          |
| (1,1006) | 1:93:A:TYR:H     | 1:93:A:TYR:HD1   | 6        | 1.24          |
| (1,1006) | 1:93:A:TYR:H     | 1:93:A:TYR:HD1   | 19       | 1.24          |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD12 | 5        | 1.24          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE2   | 2        | 1.24          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 13       | 1.23          |
| (1,1722) | 1:69:A:LEU:HD23  | 1:150:A:HIS:HE1  | 10       | 1.22          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 13       | 1.22          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 1        | 1.22          |
| (1,2011) | 1:151:A:ILE:HD12 | 1:157:A:VAL:H    | 19       | 1.21          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD22 | 9        | 1.21          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD11 | 19       | 1.21          |
| (1,1519) | 1:66:A:VAL:HG12  | 1:89:A:VAL:HG13  | 4        | 1.21          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 19       | 1.21          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1  | 8        | 1.21          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 2        | 1.2           |
| (1,1676) | 1:99:A:LEU:HD22  | 1:126:A:VAL:HB   | 18       | 1.2           |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD11 | 6        | 1.19          |
| (1,99)   | 1:160:A:GLY:H    | 1:157:A:VAL:HG13 | 10       | 1.19          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG21  | 15       | 1.19          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 1        | 1.19          |
| (1,1722) | 1:69:A:LEU:HD22  | 1:149:A:GLU:H    | 20       | 1.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 19       | 1.18          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD13 | 4        | 1.18          |
| (1,1514) | 1:147:A:ILE:HD12 | 1:157:A:VAL:H    | 4        | 1.18          |
| (1,1454) | 1:89:A:VAL:HG11  | 1:139:A:LEU:HG   | 1        | 1.18          |
| (1,1400) | 1:99:A:LEU:HD12  | 1:98:A:GLU:HB3   | 4        | 1.18          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 18       | 1.18          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 15       | 1.18          |
| (1,1722) | 1:69:A:LEU:HD23  | 1:149:A:GLU:H    | 16       | 1.16          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG23 | 3        | 1.16          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE2   | 9        | 1.16          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 14       | 1.16          |
| (1,1830) | 1:72:A:THR:HA    | 1:70:A:THR:HG22  | 3        | 1.15          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 12       | 1.15          |
| (1,1722) | 1:69:A:LEU:HD22  | 1:149:A:GLU:H    | 4        | 1.15          |
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 9        | 1.15          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG23 | 1        | 1.15          |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD11 | 11       | 1.15          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG22  | 4        | 1.15          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 2        | 1.15          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 8        | 1.14          |
| (1,1722) | 1:69:A:LEU:HD23  | 1:150:A:HIS:HE1  | 14       | 1.14          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 8        | 1.14          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 12       | 1.14          |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG13  | 6        | 1.14          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 7        | 1.14          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 1        | 1.14          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 14       | 1.14          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 6        | 1.14          |
| (1,2011) | 1:151:A:ILE:HD12 | 1:157:A:VAL:H    | 12       | 1.13          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 14       | 1.13          |
| (1,1676) | 1:99:A:LEU:HD23  | 1:126:A:VAL:HB   | 5        | 1.13          |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG12  | 3        | 1.13          |
| (1,1395) | 1:153:A:VAL:HG12 | 1:150:A:HIS:HA   | 13       | 1.13          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG21  | 10       | 1.13          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 20       | 1.13          |
| (1,1722) | 1:69:A:LEU:HD21  | 1:150:A:HIS:HE1  | 19       | 1.12          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD13 | 14       | 1.12          |
| (1,1400) | 1:99:A:LEU:HD13  | 1:98:A:GLU:HB3   | 20       | 1.12          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 7        | 1.11          |
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 4        | 1.11          |
| (1,1400) | 1:99:A:LEU:HD12  | 1:98:A:GLU:HB3   | 15       | 1.11          |
| (1,1388) | 1:95:A:LYS:HD2   | 1:77:A:ILE:HD13  | 18       | 1.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE2   | 3        | 1.11          |
| (1,1679) | 1:74:A:LEU:HD22  | 1:76:A:PRO:HG3   | 5        | 1.1           |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG23 | 11       | 1.1           |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG21  | 20       | 1.1           |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG23 | 18       | 1.1           |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD11 | 13       | 1.1           |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 2        | 1.1           |
| (1,1722) | 1:69:A:LEU:HD23  | 1:149:A:GLU:H    | 7        | 1.09          |
| (1,1557) | 1:147:A:ILE:HD13 | 1:144:A:LYS:HE2  | 11       | 1.09          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:139:A:LEU:HD13 | 18       | 1.09          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG13 | 16       | 1.09          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 10       | 1.09          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG12 | 20       | 1.09          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 15       | 1.09          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE2   | 7        | 1.09          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 9        | 1.09          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 6        | 1.08          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 1        | 1.08          |
| (1,1514) | 1:147:A:ILE:HD13 | 1:157:A:VAL:H    | 8        | 1.08          |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG12  | 1        | 1.08          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 3        | 1.08          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG12 | 14       | 1.08          |
| (1,2011) | 1:151:A:ILE:HD13 | 1:157:A:VAL:H    | 17       | 1.07          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 16       | 1.07          |
| (1,1519) | 1:66:A:VAL:HG11  | 1:89:A:VAL:HG21  | 9        | 1.07          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 14       | 1.07          |
| (1,92)   | 1:95:A:LYS:H     | 1:116:A:LEU:HD22 | 10       | 1.07          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG23  | 5        | 1.07          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE2   | 13       | 1.07          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 13       | 1.07          |
| (1,2797) | 1:150:A:HIS:HE1  | 1:98:A:GLU:HB3   | 9        | 1.06          |
| (1,1557) | 1:147:A:ILE:HD12 | 1:144:A:LYS:HE2  | 17       | 1.06          |
| (1,1514) | 1:147:A:ILE:HD11 | 1:157:A:VAL:H    | 17       | 1.06          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 2        | 1.06          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1  | 17       | 1.06          |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD11 | 14       | 1.06          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG22  | 18       | 1.06          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 17       | 1.06          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG23  | 18       | 1.06          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 11       | 1.06          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 8        | 1.06          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 17       | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 1        | 1.05          |
| (1,1514) | 1:147:A:ILE:HD13 | 1:157:A:VAL:H    | 3        | 1.05          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG12 | 8        | 1.05          |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG12  | 14       | 1.05          |
| (1,1433) | 1:117:A:LYS:HD3  | 1:116:A:LEU:HD23 | 16       | 1.05          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 9        | 1.05          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG12 | 1        | 1.05          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 15       | 1.04          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG22 | 7        | 1.04          |
| (1,112)  | 1:87:A:SER:H     | 1:130:A:ILE:HD12 | 7        | 1.04          |
| (1,1722) | 1:69:A:LEU:HD23  | 1:149:A:GLU:H    | 6        | 1.03          |
| (1,1679) | 1:74:A:LEU:HD22  | 1:76:A:PRO:HG3   | 10       | 1.03          |
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 11       | 1.03          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 17       | 1.03          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 11       | 1.03          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 11       | 1.03          |
| (1,2418) | 1:108:A:ILE:HA   | 1:90:A:TYR:HE1   | 1        | 1.02          |
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 8        | 1.02          |
| (1,1433) | 1:170:A:LYS:HD2  | 1:167:A:THR:HG23 | 5        | 1.02          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 20       | 1.02          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG22  | 1        | 1.02          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG23  | 7        | 1.02          |
| (1,1557) | 1:147:A:ILE:HD12 | 1:143:A:TRP:HB2  | 2        | 1.01          |
| (1,1543) | 1:119:A:VAL:HG11 | 1:168:A:PHE:HB3  | 17       | 1.01          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 4        | 1.01          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD23  | 5        | 1.01          |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG11  | 16       | 1.01          |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD3  | 7        | 1.01          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG22 | 19       | 1.01          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG11 | 9        | 1.01          |
| (1,1679) | 1:74:A:LEU:HD21  | 1:76:A:PRO:HG3   | 1        | 1.0           |
| (1,1514) | 1:147:A:ILE:HD13 | 1:157:A:VAL:H    | 10       | 1.0           |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 15       | 1.0           |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG22  | 1        | 1.0           |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 18       | 0.99          |
| (1,1676) | 1:69:A:LEU:HD23  | 1:149:A:GLU:HB3  | 17       | 0.99          |
| (1,1544) | 1:173:A:LEU:HD12 | 1:173:A:LEU:HA   | 16       | 0.99          |
| (1,1494) | 1:172:A:THR:HB   | 1:171:A:VAL:HG13 | 5        | 0.99          |
| (1,1400) | 1:99:A:LEU:HD13  | 1:98:A:GLU:HB3   | 17       | 0.99          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 8        | 0.99          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1  | 18       | 0.99          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 12       | 0.99          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,112)  | 1:87:A:SER:H     | 1:130:A:ILE:HD11 | 5        | 0.99          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG22  | 11       | 0.99          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE2   | 16       | 0.99          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 18       | 0.99          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 17       | 0.98          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 6        | 0.98          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:83:A:ILE:HG23  | 4        | 0.98          |
| (1,1433) | 1:117:A:LYS:HD3  | 1:116:A:LEU:HD22 | 19       | 0.98          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 5        | 0.98          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 2        | 0.98          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG23 | 11       | 0.98          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG22 | 3        | 0.98          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 4        | 0.98          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 6        | 0.98          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG11 | 13       | 0.98          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG21  | 9        | 0.98          |
| (1,2011) | 1:151:A:ILE:HD13 | 1:157:A:VAL:H    | 3        | 0.97          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 5        | 0.97          |
| (1,1519) | 1:66:A:VAL:HG11  | 1:89:A:VAL:HG21  | 10       | 0.97          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD22  | 20       | 0.97          |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG11  | 7        | 0.97          |
| (1,1426) | 1:117:A:LYS:HB2  | 1:117:A:LYS:HE3  | 14       | 0.97          |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD2  | 17       | 0.97          |
| (1,1377) | 1:89:A:VAL:HG11  | 1:66:A:VAL:HG11  | 1        | 0.97          |
| (1,676)  | 1:167:A:THR:H    | 1:168:A:PHE:HD1  | 16       | 0.97          |
| (1,363)  | 1:155:A:GLY:H    | 1:153:A:VAL:HG21 | 13       | 0.97          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 10       | 0.97          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 8        | 0.97          |
| (1,1722) | 1:69:A:LEU:HD22  | 1:149:A:GLU:H    | 13       | 0.96          |
| (1,1676) | 1:99:A:LEU:HD21  | 1:126:A:VAL:HB   | 2        | 0.96          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 5        | 0.96          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG13 | 5        | 0.96          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG22 | 14       | 0.96          |
| (1,1510) | 1:115:A:HIS:HB3  | 1:116:A:LEU:HD22 | 17       | 0.95          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG22  | 4        | 0.95          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG23  | 18       | 0.95          |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD23  | 11       | 0.94          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG22 | 17       | 0.94          |
| (1,1435) | 1:84:A:PRO:HG3   | 1:130:A:ILE:HD13 | 6        | 0.94          |
| (1,1378) | 1:136:A:LYS:HE2  | 1:136:A:LYS:HB2  | 17       | 0.94          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 12       | 0.94          |
| (1,1850) | 1:147:A:ILE:HD12 | 1:148:A:GLU:HG3  | 16       | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 2        | 0.93          |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE3  | 1        | 0.93          |
| (1,1377) | 1:89:A:VAL:HG13  | 1:131:A:VAL:HG11 | 3        | 0.93          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 13       | 0.93          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG22  | 15       | 0.93          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG13  | 2        | 0.93          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE2   | 4        | 0.93          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG23 | 15       | 0.92          |
| (1,2847) | 1:93:A:TYR:HE1   | 1:93:A:TYR:H     | 6        | 0.92          |
| (1,2847) | 1:93:A:TYR:HE1   | 1:93:A:TYR:H     | 19       | 0.92          |
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 18       | 0.92          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 6        | 0.92          |
| (1,1514) | 1:147:A:ILE:HD12 | 1:157:A:VAL:H    | 1        | 0.92          |
| (1,1400) | 1:99:A:LEU:HD12  | 1:98:A:GLU:HB3   | 14       | 0.92          |
| (1,1000) | 1:93:A:TYR:H     | 1:93:A:TYR:HE1   | 6        | 0.92          |
| (1,1000) | 1:93:A:TYR:H     | 1:93:A:TYR:HE1   | 19       | 0.92          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 5        | 0.92          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 8        | 0.92          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE2   | 12       | 0.92          |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG13  | 16       | 0.91          |
| (1,1378) | 1:136:A:LYS:HE3  | 1:136:A:LYS:HB3  | 11       | 0.91          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 19       | 0.91          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG13  | 9        | 0.91          |
| (1,1679) | 1:74:A:LEU:HD22  | 1:76:A:PRO:HG3   | 14       | 0.9           |
| (1,1557) | 1:147:A:ILE:HD11 | 1:144:A:LYS:HE2  | 15       | 0.9           |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG12  | 4        | 0.9           |
| (1,1395) | 1:153:A:VAL:HG13 | 1:150:A:HIS:HA   | 9        | 0.9           |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG23 | 19       | 0.9           |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG13  | 6        | 0.9           |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 19       | 0.9           |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 12       | 0.9           |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 10       | 0.89          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:140:A:THR:HG22 | 16       | 0.89          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 3        | 0.89          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:83:A:ILE:HG22  | 15       | 0.89          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD22  | 17       | 0.89          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG13 | 9        | 0.89          |
| (1,1377) | 1:89:A:VAL:HG13  | 1:131:A:VAL:HG12 | 16       | 0.89          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 12       | 0.89          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 9        | 0.89          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 10       | 0.89          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG22  | 17       | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG23  | 8        | 0.89          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG23  | 8        | 0.89          |
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 7        | 0.88          |
| (1,1629) | 1:77:A:ILE:HG23  | 1:78:A:THR:HA    | 4        | 0.88          |
| (1,1629) | 1:77:A:ILE:HG21  | 1:78:A:THR:HA    | 5        | 0.88          |
| (1,1388) | 1:67:A:LYS:HD3   | 1:66:A:VAL:HG11  | 5        | 0.88          |
| (1,1377) | 1:89:A:VAL:HG11  | 1:131:A:VAL:HG11 | 4        | 0.88          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 12       | 0.88          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG23 | 16       | 0.88          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG11 | 12       | 0.88          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE2   | 10       | 0.88          |
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 6        | 0.87          |
| (1,1550) | 1:72:A:THR:HG23  | 1:74:A:LEU:HD21  | 3        | 0.87          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD22  | 3        | 0.87          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD22  | 6        | 0.87          |
| (1,1400) | 1:99:A:LEU:HD12  | 1:98:A:GLU:HB3   | 12       | 0.87          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 17       | 0.87          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HD13 | 4        | 0.87          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 8        | 0.87          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG22 | 2        | 0.87          |
| (1,1952) | 1:69:A:LEU:HD13  | 1:150:A:HIS:HB2  | 4        | 0.86          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 4        | 0.86          |
| (1,1557) | 1:147:A:ILE:HD13 | 1:144:A:LYS:HE2  | 4        | 0.86          |
| (1,1542) | 1:173:A:LEU:HD21 | 1:173:A:LEU:HA   | 3        | 0.86          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 7        | 0.86          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 8        | 0.86          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 17       | 0.86          |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG22 | 11       | 0.86          |
| (1,63)   | 1:170:A:LYS:H    | 1:166:A:ASN:HB2  | 6        | 0.86          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG22  | 11       | 0.86          |
| (1,1830) | 1:72:A:THR:HA    | 1:70:A:THR:HG23  | 9        | 0.85          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:120:A:PRO:HA   | 18       | 0.85          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:140:A:THR:HG23 | 1        | 0.85          |
| (1,1550) | 1:72:A:THR:HG21  | 1:69:A:LEU:HD13  | 10       | 0.85          |
| (1,1514) | 1:147:A:ILE:HD12 | 1:157:A:VAL:H    | 18       | 0.85          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD22  | 14       | 0.85          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG12 | 4        | 0.85          |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD2  | 4        | 0.85          |
| (1,1400) | 1:99:A:LEU:HD11  | 1:98:A:GLU:HB3   | 7        | 0.85          |
| (1,1400) | 1:99:A:LEU:HD13  | 1:98:A:GLU:HB3   | 8        | 0.85          |
| (1,1388) | 1:95:A:LYS:HD2   | 1:77:A:ILE:HD13  | 19       | 0.85          |
| (1,1377) | 1:89:A:VAL:HG13  | 1:139:A:LEU:HD21 | 10       | 0.85          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 11       | 0.85          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 13       | 0.85          |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD11 | 6        | 0.85          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG21  | 16       | 0.85          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 20       | 0.85          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 3        | 0.85          |
| (1,2011) | 1:151:A:ILE:HD11 | 1:157:A:VAL:H    | 18       | 0.84          |
| (1,1831) | 1:125:A:SER:HB2  | 1:74:A:LEU:HB3   | 17       | 0.84          |
| (1,1722) | 1:69:A:LEU:HD21  | 1:150:A:HIS:HE1  | 8        | 0.84          |
| (1,1566) | 1:119:A:VAL:HG23 | 1:167:A:THR:HG21 | 12       | 0.84          |
| (1,1514) | 1:147:A:ILE:HD11 | 1:157:A:VAL:H    | 13       | 0.84          |
| (1,1456) | 1:157:A:VAL:HG21 | 1:151:A:ILE:HG13 | 14       | 0.84          |
| (1,1456) | 1:157:A:VAL:HG22 | 1:151:A:ILE:HG13 | 14       | 0.84          |
| (1,1456) | 1:157:A:VAL:HG23 | 1:151:A:ILE:HG13 | 14       | 0.84          |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD2  | 15       | 0.84          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 9        | 0.84          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 18       | 0.84          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG13 | 18       | 0.84          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 2        | 0.84          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 5        | 0.84          |
| (1,1830) | 1:72:A:THR:HA    | 1:70:A:THR:HG22  | 19       | 0.83          |
| (1,1629) | 1:77:A:ILE:HG23  | 1:78:A:THR:HA    | 19       | 0.83          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 19       | 0.83          |
| (1,1550) | 1:72:A:THR:HG23  | 1:74:A:LEU:HD22  | 7        | 0.83          |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD21  | 14       | 0.83          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 5        | 0.83          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 10       | 0.83          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 14       | 0.83          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 17       | 0.83          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG23 | 7        | 0.83          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG11 | 4        | 0.83          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG12 | 19       | 0.83          |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD23 | 10       | 0.83          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG2  | 8        | 0.83          |
| (1,2012) | 1:151:A:ILE:HG23 | 1:151:A:ILE:H    | 4        | 0.82          |
| (1,2011) | 1:151:A:ILE:HD11 | 1:157:A:VAL:H    | 5        | 0.82          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 3        | 0.82          |
| (1,1831) | 1:125:A:SER:HB2  | 1:74:A:LEU:HB3   | 15       | 0.82          |
| (1,1629) | 1:77:A:ILE:HG21  | 1:78:A:THR:HA    | 14       | 0.82          |
| (1,1506) | 1:156:A:LYS:HE3  | 1:157:A:VAL:H    | 17       | 0.82          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG13 | 2        | 0.82          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 9        | 0.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG23 | 15       | 0.82          |
| (1,85)   | 1:125:A:SER:H    | 1:95:A:LYS:HB3   | 9        | 0.82          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG22  | 9        | 0.82          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 12       | 0.82          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG22  | 14       | 0.82          |
| (1,2012) | 1:151:A:ILE:HG22 | 1:151:A:ILE:H    | 8        | 0.81          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 12       | 0.81          |
| (1,1722) | 1:69:A:LEU:HD22  | 1:150:A:HIS:HE1  | 2        | 0.81          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 8        | 0.81          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 17       | 0.81          |
| (1,1514) | 1:147:A:ILE:HD13 | 1:157:A:VAL:H    | 9        | 0.81          |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE3  | 12       | 0.81          |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG23 | 19       | 0.81          |
| (1,2012) | 1:151:A:ILE:HG23 | 1:151:A:ILE:H    | 9        | 0.8           |
| (1,2012) | 1:151:A:ILE:HG21 | 1:151:A:ILE:H    | 13       | 0.8           |
| (1,1676) | 1:69:A:LEU:HD22  | 1:149:A:GLU:HB3  | 13       | 0.8           |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 10       | 0.8           |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB1  | 17       | 0.8           |
| (1,1557) | 1:147:A:ILE:HD12 | 1:144:A:LYS:HE2  | 16       | 0.8           |
| (1,1550) | 1:72:A:THR:HG22  | 1:74:A:LEU:HD22  | 8        | 0.8           |
| (1,1390) | 1:152:A:LYS:HE2  | 1:149:A:GLU:HB3  | 17       | 0.8           |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 15       | 0.8           |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 9        | 0.8           |
| (1,363)  | 1:155:A:GLY:H    | 1:154:A:THR:HG23 | 18       | 0.8           |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG21 | 5        | 0.8           |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG22 | 18       | 0.8           |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG21  | 20       | 0.8           |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 7        | 0.8           |
| (1,2012) | 1:151:A:ILE:HG21 | 1:151:A:ILE:H    | 5        | 0.79          |
| (1,2012) | 1:151:A:ILE:HG22 | 1:151:A:ILE:H    | 6        | 0.79          |
| (1,2012) | 1:151:A:ILE:HG22 | 1:151:A:ILE:H    | 19       | 0.79          |
| (1,1850) | 1:147:A:ILE:HD12 | 1:148:A:GLU:HG3  | 14       | 0.79          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:140:A:THR:HG22 | 9        | 0.79          |
| (1,1455) | 1:170:A:LYS:HG2  | 1:171:A:VAL:HA   | 15       | 0.79          |
| (1,1400) | 1:99:A:LEU:HD12  | 1:98:A:GLU:HB3   | 16       | 0.79          |
| (1,1400) | 1:99:A:LEU:HD12  | 1:98:A:GLU:HB3   | 19       | 0.79          |
| (1,363)  | 1:155:A:GLY:H    | 1:154:A:THR:HG23 | 2        | 0.79          |
| (1,363)  | 1:155:A:GLY:H    | 1:153:A:VAL:HG21 | 9        | 0.79          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 11       | 0.79          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG11 | 10       | 0.79          |
| (1,15)   | 1:143:A:TRP:HE1  | 1:90:A:TYR:HE1   | 4        | 0.79          |
| (1,2799) | 1:93:A:TYR:HE1   | 1:69:A:LEU:HD13  | 20       | 0.78          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2012) | 1:151:A:ILE:HG21 | 1:151:A:ILE:H    | 12       | 0.78          |
| (1,2012) | 1:151:A:ILE:HG21 | 1:151:A:ILE:H    | 15       | 0.78          |
| (1,2012) | 1:151:A:ILE:HG23 | 1:151:A:ILE:H    | 17       | 0.78          |
| (1,1956) | 1:69:A:LEU:HD13  | 1:69:A:LEU:HA    | 1        | 0.78          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 11       | 0.78          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:140:A:THR:HG23 | 12       | 0.78          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 14       | 0.78          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD23  | 12       | 0.78          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 2        | 0.78          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 20       | 0.78          |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG21 | 7        | 0.78          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 5        | 0.78          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG23 | 11       | 0.78          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 18       | 0.78          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG22 | 5        | 0.77          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG21 | 19       | 0.77          |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 6        | 0.77          |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 10       | 0.77          |
| (1,2797) | 1:150:A:HIS:HE1  | 1:153:A:VAL:HB   | 19       | 0.77          |
| (1,2012) | 1:151:A:ILE:HG21 | 1:151:A:ILE:H    | 1        | 0.77          |
| (1,2012) | 1:151:A:ILE:HG22 | 1:151:A:ILE:H    | 2        | 0.77          |
| (1,1956) | 1:69:A:LEU:HD13  | 1:69:A:LEU:HA    | 17       | 0.77          |
| (1,1807) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 8        | 0.77          |
| (1,1668) | 1:140:A:THR:HG21 | 1:140:A:THR:H    | 2        | 0.77          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB1  | 3        | 0.77          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB2  | 5        | 0.77          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG21 | 10       | 0.77          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG13 | 17       | 0.77          |
| (1,1420) | 1:87:A:SER:HB3   | 1:106:A:ARG:HG2  | 18       | 0.77          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 4        | 0.77          |
| (1,368)  | 1:122:A:LEU:H    | 1:122:A:LEU:HD13 | 18       | 0.77          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG21 | 2        | 0.77          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG21  | 1        | 0.77          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 5        | 0.77          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE2   | 14       | 0.77          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG12 | 8        | 0.77          |
| (1,2012) | 1:151:A:ILE:HG22 | 1:151:A:ILE:H    | 14       | 0.76          |
| (1,1956) | 1:69:A:LEU:HD12  | 1:69:A:LEU:HA    | 7        | 0.76          |
| (1,1956) | 1:69:A:LEU:HD13  | 1:69:A:LEU:HA    | 9        | 0.76          |
| (1,1956) | 1:69:A:LEU:HD13  | 1:69:A:LEU:HA    | 12       | 0.76          |
| (1,1956) | 1:69:A:LEU:HD11  | 1:69:A:LEU:HA    | 18       | 0.76          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 20       | 0.76          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 8        | 0.76          |
| (1,1807) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 9        | 0.76          |
| (1,1668) | 1:140:A:THR:HG23 | 1:140:A:THR:H    | 19       | 0.76          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB1  | 13       | 0.76          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD22  | 18       | 0.76          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG11 | 1        | 0.76          |
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE2  | 6        | 0.76          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 20       | 0.76          |
| (1,363)  | 1:155:A:GLY:H    | 1:153:A:VAL:HG23 | 20       | 0.76          |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG22 | 3        | 0.76          |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG23 | 18       | 0.76          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG23 | 19       | 0.76          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG13 | 9        | 0.76          |
| (1,1956) | 1:69:A:LEU:HD11  | 1:69:A:LEU:HA    | 5        | 0.75          |
| (1,1956) | 1:69:A:LEU:HD13  | 1:69:A:LEU:HA    | 6        | 0.75          |
| (1,1956) | 1:69:A:LEU:HD11  | 1:69:A:LEU:HA    | 14       | 0.75          |
| (1,1956) | 1:69:A:LEU:HD13  | 1:69:A:LEU:HA    | 19       | 0.75          |
| (1,1878) | 1:147:A:ILE:HG22 | 1:148:A:GLU:HB2  | 19       | 0.75          |
| (1,1830) | 1:72:A:THR:HA    | 1:69:A:LEU:HB2   | 10       | 0.75          |
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 6        | 0.75          |
| (1,1722) | 1:69:A:LEU:HD21  | 1:150:A:HIS:HE1  | 5        | 0.75          |
| (1,1679) | 1:74:A:LEU:HD23  | 1:76:A:PRO:HG3   | 3        | 0.75          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 6        | 0.75          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 9        | 0.75          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 16       | 0.75          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 20       | 0.75          |
| (1,1557) | 1:147:A:ILE:HD11 | 1:144:A:LYS:HE2  | 8        | 0.75          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 19       | 0.75          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD23  | 9        | 0.75          |
| (1,1476) | 1:66:A:VAL:HG11  | 1:71:A:GLU:HG3   | 10       | 0.75          |
| (1,1476) | 1:66:A:VAL:HG12  | 1:71:A:GLU:HG3   | 10       | 0.75          |
| (1,1476) | 1:66:A:VAL:HG13  | 1:71:A:GLU:HG3   | 10       | 0.75          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 18       | 0.75          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG13 | 3        | 0.75          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 8        | 0.75          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG13 | 5        | 0.75          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 9        | 0.75          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 2        | 0.75          |
| (1,1956) | 1:69:A:LEU:HD11  | 1:69:A:LEU:HA    | 2        | 0.74          |
| (1,1824) | 1:147:A:ILE:HD13 | 1:147:A:ILE:HA   | 14       | 0.74          |
| (1,1807) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 18       | 0.74          |
| (1,1722) | 1:69:A:LEU:HD23  | 1:150:A:HIS:HE1  | 17       | 0.74          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 7        | 0.74          |
| (1,1629) | 1:77:A:ILE:HG23  | 1:120:A:PRO:HA   | 20       | 0.74          |
| (1,1550) | 1:72:A:THR:HG23  | 1:74:A:LEU:HD22  | 6        | 0.74          |
| (1,1539) | 1:69:A:LEU:HD12  | 1:149:A:GLU:HA   | 4        | 0.74          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 7        | 0.74          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 20       | 0.74          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 11       | 0.74          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 6        | 0.74          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 20       | 0.74          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG2  | 9        | 0.74          |
| (1,63)   | 1:170:A:LYS:H    | 1:166:A:ASN:HB2  | 10       | 0.74          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG13 | 18       | 0.74          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 11       | 0.74          |
| (1,2012) | 1:151:A:ILE:HG23 | 1:151:A:ILE:H    | 18       | 0.73          |
| (1,1956) | 1:69:A:LEU:HD12  | 1:69:A:LEU:HA    | 8        | 0.73          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 19       | 0.73          |
| (1,1824) | 1:147:A:ILE:HD11 | 1:147:A:ILE:HA   | 4        | 0.73          |
| (1,1824) | 1:147:A:ILE:HD13 | 1:147:A:ILE:HA   | 16       | 0.73          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 15       | 0.73          |
| (1,1668) | 1:140:A:THR:HG23 | 1:140:A:THR:H    | 13       | 0.73          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 1        | 0.73          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 2        | 0.73          |
| (1,1566) | 1:119:A:VAL:HG21 | 1:167:A:THR:HG23 | 11       | 0.73          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG11 | 12       | 0.73          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG13 | 20       | 0.73          |
| (1,678)  | 1:104:A:ILE:H    | 1:90:A:TYR:HE1   | 3        | 0.73          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 2        | 0.73          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 4        | 0.73          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 12       | 0.73          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG23 | 13       | 0.73          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG21 | 20       | 0.73          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 7        | 0.73          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG11 | 6        | 0.73          |
| (1,2012) | 1:151:A:ILE:HG23 | 1:151:A:ILE:H    | 11       | 0.72          |
| (1,1956) | 1:69:A:LEU:HD13  | 1:69:A:LEU:HA    | 15       | 0.72          |
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 15       | 0.72          |
| (1,1824) | 1:147:A:ILE:HD11 | 1:147:A:ILE:HA   | 20       | 0.72          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 10       | 0.72          |
| (1,1807) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 20       | 0.72          |
| (1,1722) | 1:69:A:LEU:HD22  | 1:150:A:HIS:HE1  | 18       | 0.72          |
| (1,1668) | 1:172:A:THR:HG21 | 1:172:A:THR:H    | 4        | 0.72          |
| (1,1668) | 1:140:A:THR:HG21 | 1:140:A:THR:H    | 9        | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1668) | 1:140:A:THR:HG22 | 1:140:A:THR:H    | 17       | 0.72          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:78:A:THR:HA    | 13       | 0.72          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 4        | 0.72          |
| (1,1476) | 1:66:A:VAL:HG21  | 1:71:A:GLU:HG3   | 8        | 0.72          |
| (1,1476) | 1:66:A:VAL:HG22  | 1:71:A:GLU:HG3   | 8        | 0.72          |
| (1,1476) | 1:66:A:VAL:HG23  | 1:71:A:GLU:HG3   | 8        | 0.72          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG11 | 10       | 0.72          |
| (1,1378) | 1:117:A:LYS:HE3  | 1:117:A:LYS:HB3  | 18       | 0.72          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 6        | 0.72          |
| (1,159)  | 1:153:A:VAL:H    | 1:153:A:VAL:HG21 | 2        | 0.72          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG21 | 17       | 0.72          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG21 | 9        | 0.72          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 17       | 0.72          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG12 | 11       | 0.72          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 4        | 0.72          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 15       | 0.72          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG13 | 14       | 0.72          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG12 | 15       | 0.72          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG13 | 17       | 0.72          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG13 | 20       | 0.72          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 14       | 0.72          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG21 | 1        | 0.71          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HB   | 16       | 0.71          |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 18       | 0.71          |
| (1,2014) | 1:77:A:ILE:HD12  | 1:126:A:VAL:HB   | 20       | 0.71          |
| (1,2012) | 1:151:A:ILE:HG22 | 1:151:A:ILE:H    | 7        | 0.71          |
| (1,1956) | 1:69:A:LEU:HD11  | 1:69:A:LEU:HA    | 11       | 0.71          |
| (1,1824) | 1:147:A:ILE:HD13 | 1:147:A:ILE:HA   | 17       | 0.71          |
| (1,1807) | 1:112:A:VAL:HG12 | 1:112:A:VAL:H    | 4        | 0.71          |
| (1,1807) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 16       | 0.71          |
| (1,1668) | 1:140:A:THR:HG23 | 1:140:A:THR:H    | 8        | 0.71          |
| (1,1668) | 1:140:A:THR:HG21 | 1:140:A:THR:H    | 16       | 0.71          |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD23  | 1        | 0.71          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG21 | 7        | 0.71          |
| (1,1544) | 1:173:A:LEU:HD12 | 1:173:A:LEU:HA   | 19       | 0.71          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 20       | 0.71          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 19       | 0.71          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG22 | 8        | 0.71          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 7        | 0.71          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG23 | 15       | 0.71          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG21 | 3        | 0.71          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 5        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 7        | 0.71          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG23 | 8        | 0.71          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG21 | 16       | 0.71          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG23 | 6        | 0.71          |
| (1,43)   | 1:146:A:TRP:H    | 1:149:A:GLU:HG2  | 2        | 0.71          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 12       | 0.71          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG21  | 12       | 0.71          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG12 | 4        | 0.71          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG12 | 19       | 0.71          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD11  | 12       | 0.71          |
| (1,2011) | 1:151:A:ILE:HD13 | 1:156:A:LYS:H    | 9        | 0.7           |
| (1,1878) | 1:147:A:ILE:HG23 | 1:148:A:GLU:HB2  | 20       | 0.7           |
| (1,1859) | 1:77:A:ILE:HD11  | 1:76:A:PRO:HB2   | 14       | 0.7           |
| (1,1831) | 1:125:A:SER:HB2  | 1:74:A:LEU:HB3   | 13       | 0.7           |
| (1,1824) | 1:147:A:ILE:HD11 | 1:147:A:ILE:HA   | 1        | 0.7           |
| (1,1722) | 1:69:A:LEU:HD21  | 1:149:A:GLU:H    | 3        | 0.7           |
| (1,1668) | 1:140:A:THR:HG21 | 1:140:A:THR:H    | 18       | 0.7           |
| (1,1629) | 1:77:A:ILE:HG23  | 1:78:A:THR:HA    | 12       | 0.7           |
| (1,1400) | 1:99:A:LEU:HD12  | 1:149:A:GLU:HG3  | 9        | 0.7           |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 11       | 0.7           |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG21 | 15       | 0.7           |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG21 | 18       | 0.7           |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG13 | 17       | 0.7           |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD12 | 2        | 0.7           |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG21 | 10       | 0.7           |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 2        | 0.7           |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 9        | 0.7           |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 18       | 0.7           |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD13  | 6        | 0.7           |
| (1,1843) | 1:147:A:ILE:HD12 | 1:102:A:VAL:HB   | 15       | 0.69          |
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 7        | 0.69          |
| (1,1824) | 1:147:A:ILE:HD13 | 1:147:A:ILE:HA   | 12       | 0.69          |
| (1,1668) | 1:140:A:THR:HG22 | 1:140:A:THR:H    | 1        | 0.69          |
| (1,1668) | 1:140:A:THR:HG23 | 1:140:A:THR:H    | 14       | 0.69          |
| (1,1629) | 1:77:A:ILE:HG22  | 1:120:A:PRO:HA   | 15       | 0.69          |
| (1,1544) | 1:173:A:LEU:HD12 | 1:173:A:LEU:HA   | 10       | 0.69          |
| (1,1514) | 1:147:A:ILE:HD11 | 1:157:A:VAL:H    | 12       | 0.69          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 9        | 0.69          |
| (1,1382) | 1:170:A:LYS:HB3  | 1:170:A:LYS:HE3  | 13       | 0.69          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 2        | 0.69          |
| (1,363)  | 1:155:A:GLY:H    | 1:153:A:VAL:HG22 | 4        | 0.69          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG23 | 9        | 0.69          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG22 | 20       | 0.69          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 1        | 0.69          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG23 | 14       | 0.69          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG23  | 20       | 0.69          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 5        | 0.69          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 14       | 0.69          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 17       | 0.69          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 10       | 0.69          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG12 | 7        | 0.69          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG12 | 11       | 0.69          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 4        | 0.69          |
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 9        | 0.68          |
| (1,1824) | 1:147:A:ILE:HD11 | 1:147:A:ILE:HA   | 11       | 0.68          |
| (1,1807) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 2        | 0.68          |
| (1,1807) | 1:112:A:VAL:HG13 | 1:112:A:VAL:H    | 13       | 0.68          |
| (1,1807) | 1:154:A:THR:HG22 | 1:155:A:GLY:H    | 19       | 0.68          |
| (1,1668) | 1:140:A:THR:HG22 | 1:140:A:THR:H    | 6        | 0.68          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD23  | 19       | 0.68          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 13       | 0.68          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 13       | 0.68          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 13       | 0.68          |
| (1,1415) | 1:72:A:THR:HA    | 1:127:A:LYS:HB2  | 19       | 0.68          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 11       | 0.68          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 16       | 0.68          |
| (1,535)  | 1:125:A:SER:H    | 1:93:A:TYR:HD1   | 19       | 0.68          |
| (1,363)  | 1:155:A:GLY:H    | 1:154:A:THR:HG22 | 19       | 0.68          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG21 | 13       | 0.68          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG22 | 14       | 0.68          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG22 | 6        | 0.68          |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD12 | 9        | 0.68          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG21 | 3        | 0.68          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG22  | 14       | 0.68          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 11       | 0.68          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG11 | 1        | 0.68          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG13 | 2        | 0.68          |
| (1,18)   | 1:112:A:VAL:H    | 1:112:A:VAL:HG11 | 12       | 0.68          |
| (1,18)   | 1:112:A:VAL:H    | 1:83:A:ILE:HG21  | 16       | 0.68          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 8        | 0.68          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD13  | 17       | 0.68          |
| (1,1984) | 1:69:A:LEU:HD12  | 1:151:A:ILE:H    | 20       | 0.67          |
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 3        | 0.67          |
| (1,1824) | 1:147:A:ILE:HD11 | 1:147:A:ILE:HA   | 5        | 0.67          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1824) | 1:147:A:ILE:HD11 | 1:147:A:ILE:HA   | 19       | 0.67          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 3        | 0.67          |
| (1,1679) | 1:74:A:LEU:HD22  | 1:76:A:PRO:HG3   | 16       | 0.67          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 7        | 0.67          |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG22  | 11       | 0.67          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 2        | 0.67          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 4        | 0.67          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG12 | 11       | 0.67          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 4        | 0.67          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 4        | 0.67          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 4        | 0.67          |
| (1,1391) | 1:162:A:LYS:HB2  | 1:162:A:LYS:HE2  | 14       | 0.67          |
| (1,1377) | 1:89:A:VAL:HG22  | 1:131:A:VAL:HG12 | 9        | 0.67          |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 16       | 0.67          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD11 | 8        | 0.67          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD12 | 8        | 0.67          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD13 | 8        | 0.67          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG11 | 6        | 0.67          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG12 | 6        | 0.67          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG13 | 6        | 0.67          |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG11 | 16       | 0.67          |
| (1,92)   | 1:95:A:LYS:H     | 1:122:A:LEU:HD12 | 3        | 0.67          |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG21 | 20       | 0.67          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG22  | 13       | 0.67          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 16       | 0.67          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG2  | 16       | 0.67          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 1        | 0.67          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 3        | 0.67          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 13       | 0.67          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 17       | 0.67          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 1        | 0.67          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD13  | 2        | 0.67          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD11  | 16       | 0.67          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD11  | 19       | 0.67          |
| (1,2799) | 1:93:A:TYR:HE2   | 1:69:A:LEU:HD13  | 3        | 0.66          |
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 2        | 0.66          |
| (1,1824) | 1:147:A:ILE:HD11 | 1:147:A:ILE:HA   | 18       | 0.66          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 1        | 0.66          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 1        | 0.66          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 1        | 0.66          |
| (1,1577) | 1:150:A:HIS:HB3  | 1:154:A:THR:HG22 | 3        | 0.66          |
| (1,1544) | 1:173:A:LEU:HD12 | 1:173:A:LEU:HA   | 1        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 11       | 0.66          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD23  | 1        | 0.66          |
| (1,1485) | 1:85:A:SER:HB3   | 1:84:A:PRO:HB2   | 1        | 0.66          |
| (1,1433) | 1:136:A:LYS:HD2  | 1:104:A:ILE:HG21 | 15       | 0.66          |
| (1,1382) | 1:170:A:LYS:HB3  | 1:170:A:LYS:HE3  | 5        | 0.66          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG11 | 1        | 0.66          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG12 | 1        | 0.66          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG13 | 1        | 0.66          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 4        | 0.66          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 4        | 0.66          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 4        | 0.66          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 14       | 0.66          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 3        | 0.66          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 15       | 0.66          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG21  | 19       | 0.66          |
| (1,20)   | 1:113:A:SER:H    | 1:90:A:TYR:HE1   | 5        | 0.66          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 13       | 0.66          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD11  | 15       | 0.66          |
| (1,2014) | 1:77:A:ILE:HD13  | 1:76:A:PRO:HG2   | 2        | 0.65          |
| (1,2011) | 1:151:A:ILE:HD13 | 1:157:A:VAL:H    | 10       | 0.65          |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 10       | 0.65          |
| (1,1550) | 1:72:A:THR:HG23  | 1:74:A:LEU:HD23  | 12       | 0.65          |
| (1,1544) | 1:173:A:LEU:HD12 | 1:173:A:LEU:HA   | 11       | 0.65          |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG22  | 4        | 0.65          |
| (1,1510) | 1:115:A:HIS:HB3  | 1:116:A:LEU:HD23 | 7        | 0.65          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD21  | 16       | 0.65          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 15       | 0.65          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 15       | 0.65          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 15       | 0.65          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 13       | 0.65          |
| (1,132)  | 1:127:A:LYS:H    | 1:108:A:ILE:HG23 | 1        | 0.65          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 4        | 0.65          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 4        | 0.65          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG2  | 16       | 0.65          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 19       | 0.65          |
| (1,2012) | 1:151:A:ILE:HG21 | 1:155:A:GLY:H    | 10       | 0.64          |
| (1,1824) | 1:147:A:ILE:HD12 | 1:147:A:ILE:HA   | 10       | 0.64          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 6        | 0.64          |
| (1,1577) | 1:150:A:HIS:HB3  | 1:154:A:THR:HG22 | 11       | 0.64          |
| (1,1550) | 1:72:A:THR:HG21  | 1:69:A:LEU:HD13  | 5        | 0.64          |
| (1,1420) | 1:87:A:SER:HB3   | 1:106:A:ARG:HB2  | 2        | 0.64          |
| (1,1400) | 1:99:A:LEU:HD11  | 1:98:A:GLU:HB3   | 1        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1378) | 1:117:A:LYS:HE3  | 1:117:A:LYS:HB3  | 9        | 0.64          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG11  | 9        | 0.64          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG12  | 9        | 0.64          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG13  | 9        | 0.64          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 11       | 0.64          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG21 | 4        | 0.64          |
| (1,71)   | 1:71:A:GLU:H     | 1:69:A:LEU:HG    | 11       | 0.64          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG2  | 19       | 0.64          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 12       | 0.64          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 13       | 0.64          |
| (1,18)   | 1:112:A:VAL:H    | 1:83:A:ILE:HG23  | 3        | 0.64          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD11  | 3        | 0.64          |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 3        | 0.63          |
| (1,1861) | 1:104:A:ILE:HD11 | 1:140:A:THR:H    | 10       | 0.63          |
| (1,1676) | 1:69:A:LEU:HD23  | 1:149:A:GLU:HB3  | 11       | 0.63          |
| (1,1668) | 1:140:A:THR:HG23 | 1:140:A:THR:H    | 10       | 0.63          |
| (1,1666) | 1:156:A:LYS:HG2  | 1:155:A:GLY:H    | 12       | 0.63          |
| (1,1612) | 1:148:A:GLU:HG2  | 1:152:A:LYS:HE2  | 14       | 0.63          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 15       | 0.63          |
| (1,1519) | 1:66:A:VAL:HG12  | 1:89:A:VAL:HG22  | 5        | 0.63          |
| (1,1504) | 1:147:A:ILE:HD12 | 1:102:A:VAL:HG23 | 2        | 0.63          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 17       | 0.63          |
| (1,1390) | 1:152:A:LYS:HE2  | 1:148:A:GLU:HB3  | 14       | 0.63          |
| (1,1382) | 1:170:A:LYS:HB2  | 1:170:A:LYS:HE2  | 7        | 0.63          |
| (1,1382) | 1:117:A:LYS:HB3  | 1:117:A:LYS:HE3  | 20       | 0.63          |
| (1,346)  | 1:155:A:GLY:H    | 1:156:A:LYS:HG2  | 12       | 0.63          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 1        | 0.63          |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG3  | 6        | 0.63          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG11 | 7        | 0.63          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG12 | 7        | 0.63          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG13 | 7        | 0.63          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG11  | 16       | 0.63          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG12  | 16       | 0.63          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG13  | 16       | 0.63          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG21 | 14       | 0.63          |
| (1,117)  | 1:140:A:THR:H    | 1:140:A:THR:HG23 | 10       | 0.63          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 17       | 0.63          |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG22 | 7        | 0.63          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 8        | 0.63          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG3  | 10       | 0.63          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 20       | 0.63          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG2  | 8        | 0.63          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 17       | 0.63          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 18       | 0.63          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 20       | 0.63          |
| (1,2798) | 1:93:A:TYR:HE1   | 1:102:A:VAL:HG11 | 10       | 0.62          |
| (1,2797) | 1:150:A:HIS:HE1  | 1:153:A:VAL:HB   | 8        | 0.62          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 16       | 0.62          |
| (1,1770) | 1:98:A:GLU:HB2   | 1:100:A:GLN:HE22 | 5        | 0.62          |
| (1,1566) | 1:119:A:VAL:HG21 | 1:167:A:THR:HG22 | 20       | 0.62          |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD22  | 2        | 0.62          |
| (1,1506) | 1:170:A:LYS:HE2  | 1:171:A:VAL:H    | 2        | 0.62          |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 12       | 0.62          |
| (1,1485) | 1:85:A:SER:HB3   | 1:84:A:PRO:HB2   | 19       | 0.62          |
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE3  | 12       | 0.62          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 20       | 0.62          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 20       | 0.62          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 20       | 0.62          |
| (1,1420) | 1:87:A:SER:HB3   | 1:106:A:ARG:HB2  | 16       | 0.62          |
| (1,1402) | 1:112:A:VAL:HA   | 1:115:A:HIS:HD2  | 7        | 0.62          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 1        | 0.62          |
| (1,302)  | 1:146:A:TRP:HE1  | 1:69:A:LEU:HB3   | 13       | 0.62          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 2        | 0.62          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 2        | 0.62          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 2        | 0.62          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 9        | 0.62          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 9        | 0.62          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 9        | 0.62          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 8        | 0.62          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG21 | 7        | 0.62          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 3        | 0.62          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 14       | 0.62          |
| (1,2014) | 1:77:A:ILE:HD12  | 1:126:A:VAL:HB   | 17       | 0.61          |
| (1,2012) | 1:151:A:ILE:HG22 | 1:155:A:GLY:H    | 3        | 0.61          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 10       | 0.61          |
| (1,1826) | 1:167:A:THR:HA   | 1:170:A:LYS:HB3  | 4        | 0.61          |
| (1,1824) | 1:147:A:ILE:HD13 | 1:147:A:ILE:HA   | 13       | 0.61          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE3   | 3        | 0.61          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB1  | 11       | 0.61          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG23 | 17       | 0.61          |
| (1,1547) | 1:135:A:ASP:HB2  | 1:131:A:VAL:HG23 | 16       | 0.61          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 18       | 0.61          |
| (1,1455) | 1:170:A:LYS:HG3  | 1:171:A:VAL:HA   | 10       | 0.61          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 12       | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 12       | 0.61          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 12       | 0.61          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 16       | 0.61          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 16       | 0.61          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 16       | 0.61          |
| (1,1420) | 1:87:A:SER:HB3   | 1:106:A:ARG:HB2  | 12       | 0.61          |
| (1,1402) | 1:112:A:VAL:HA   | 1:115:A:HIS:HD2  | 13       | 0.61          |
| (1,363)  | 1:155:A:GLY:H    | 1:153:A:VAL:HG22 | 16       | 0.61          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 14       | 0.61          |
| (1,84)   | 1:72:A:THR:H     | 1:69:A:LEU:HG    | 12       | 0.61          |
| (1,71)   | 1:71:A:GLU:H     | 1:69:A:LEU:HG    | 8        | 0.61          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 4        | 0.61          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 16       | 0.61          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 6        | 0.61          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HG3   | 8        | 0.61          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 4        | 0.61          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 7        | 0.61          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 19       | 0.61          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD11  | 5        | 0.61          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 14       | 0.6           |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 1        | 0.6           |
| (1,1953) | 1:83:A:ILE:HG21  | 1:128:A:VAL:HA   | 8        | 0.6           |
| (1,1878) | 1:147:A:ILE:HG22 | 1:148:A:GLU:HB2  | 7        | 0.6           |
| (1,1843) | 1:147:A:ILE:HD11 | 1:102:A:VAL:HB   | 20       | 0.6           |
| (1,1510) | 1:115:A:HIS:HB3  | 1:167:A:THR:HG23 | 10       | 0.6           |
| (1,1506) | 1:156:A:LYS:HE2  | 1:157:A:VAL:H    | 8        | 0.6           |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 13       | 0.6           |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 5        | 0.6           |
| (1,1485) | 1:85:A:SER:HB3   | 1:84:A:PRO:HB2   | 15       | 0.6           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 6        | 0.6           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 6        | 0.6           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 6        | 0.6           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 10       | 0.6           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 10       | 0.6           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 10       | 0.6           |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD2  | 14       | 0.6           |
| (1,1382) | 1:117:A:LYS:HB3  | 1:117:A:LYS:HE3  | 16       | 0.6           |
| (1,1378) | 1:136:A:LYS:HE2  | 1:136:A:LYS:HB2  | 12       | 0.6           |
| (1,1227) | 1:168:A:PHE:H    | 1:168:A:PHE:HD1  | 18       | 0.6           |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HD13 | 2        | 0.6           |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD11 | 6        | 0.6           |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD12 | 6        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD13 | 6        | 0.6           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG11 | 3        | 0.6           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG12 | 3        | 0.6           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG13 | 3        | 0.6           |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG21 | 16       | 0.6           |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG12 | 14       | 0.6           |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 1        | 0.6           |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG23 | 8        | 0.6           |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 6        | 0.6           |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 17       | 0.6           |
| (1,18)   | 1:112:A:VAL:H    | 1:83:A:ILE:HG22  | 13       | 0.6           |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD11  | 10       | 0.6           |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 18       | 0.59          |
| (1,2799) | 1:93:A:TYR:HE2   | 1:69:A:LEU:HD13  | 4        | 0.59          |
| (1,2011) | 1:151:A:ILE:HD13 | 1:157:A:VAL:H    | 15       | 0.59          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 7        | 0.59          |
| (1,1668) | 1:172:A:THR:HG21 | 1:172:A:THR:H    | 12       | 0.59          |
| (1,1645) | 1:108:A:ILE:HG22 | 1:84:A:PRO:HD2   | 2        | 0.59          |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 10       | 0.59          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 8        | 0.59          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 8        | 0.59          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 8        | 0.59          |
| (1,1382) | 1:117:A:LYS:HB3  | 1:117:A:LYS:HE3  | 10       | 0.59          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD21 | 15       | 0.59          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 13       | 0.59          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD21 | 12       | 0.59          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD22 | 12       | 0.59          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD23 | 12       | 0.59          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 14       | 0.59          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 14       | 0.59          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 14       | 0.59          |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG13 | 2        | 0.59          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG3  | 20       | 0.59          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 7        | 0.59          |
| (1,43)   | 1:146:A:TRP:H    | 1:149:A:GLU:HG2  | 10       | 0.59          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG2  | 20       | 0.59          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG23  | 3        | 0.59          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 12       | 0.59          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 13       | 0.59          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 16       | 0.59          |
| (1,2014) | 1:77:A:ILE:HD11  | 1:126:A:VAL:HB   | 15       | 0.58          |
| (1,1963) | 1:154:A:THR:HB   | 1:156:A:LYS:HE3  | 6        | 0.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 20       | 0.58          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 20       | 0.58          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 20       | 0.58          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 18       | 0.58          |
| (1,1544) | 1:173:A:LEU:HD13 | 1:173:A:LEU:HA   | 15       | 0.58          |
| (1,1500) | 1:151:A:ILE:HG23 | 1:150:A:HIS:HB2  | 5        | 0.58          |
| (1,1402) | 1:112:A:VAL:HA   | 1:115:A:HIS:HD2  | 3        | 0.58          |
| (1,1378) | 1:136:A:LYS:HE2  | 1:136:A:LYS:HB2  | 3        | 0.58          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 17       | 0.58          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD11 | 3        | 0.58          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD12 | 3        | 0.58          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD13 | 3        | 0.58          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 18       | 0.58          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG23  | 7        | 0.58          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 6        | 0.58          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 12       | 0.58          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 1        | 0.58          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 15       | 0.58          |
| (1,8)    | 1:82:A:SER:H     | 1:83:A:ILE:HD12  | 7        | 0.58          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 18       | 0.58          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 15       | 0.57          |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 13       | 0.57          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 1        | 0.57          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD11  | 19       | 0.57          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD12  | 19       | 0.57          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD13  | 19       | 0.57          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 8        | 0.57          |
| (1,1485) | 1:85:A:SER:HB3   | 1:84:A:PRO:HB2   | 20       | 0.57          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 18       | 0.57          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 18       | 0.57          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 18       | 0.57          |
| (1,1402) | 1:112:A:VAL:HA   | 1:90:A:TYR:HE1   | 1        | 0.57          |
| (1,1382) | 1:170:A:LYS:HB2  | 1:170:A:LYS:HE2  | 6        | 0.57          |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG3  | 11       | 0.57          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG22 | 12       | 0.57          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG23 | 16       | 0.57          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 19       | 0.57          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG23 | 9        | 0.57          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 1        | 0.57          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HG3   | 5        | 0.57          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 20       | 0.57          |
| (1,2012) | 1:151:A:ILE:HG22 | 1:155:A:GLY:H    | 16       | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1901) | 1:77:A:ILE:HA    | 1:77:A:ILE:HG13  | 17       | 0.56          |
| (1,1843) | 1:147:A:ILE:HD12 | 1:102:A:VAL:HB   | 9        | 0.56          |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 9        | 0.56          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 14       | 0.56          |
| (1,1801) | 1:159:A:PRO:HG3  | 1:162:A:LYS:HE2  | 15       | 0.56          |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 11       | 0.56          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB2  | 15       | 0.56          |
| (1,1566) | 1:119:A:VAL:HG23 | 1:167:A:THR:HG23 | 18       | 0.56          |
| (1,1510) | 1:115:A:HIS:HB3  | 1:116:A:LEU:HD23 | 5        | 0.56          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD21  | 11       | 0.56          |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 19       | 0.56          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 3        | 0.56          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 16       | 0.56          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 2        | 0.56          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 2        | 0.56          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 2        | 0.56          |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE3  | 5        | 0.56          |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE2  | 8        | 0.56          |
| (1,1395) | 1:153:A:VAL:HG13 | 1:150:A:HIS:HA   | 16       | 0.56          |
| (1,1382) | 1:170:A:LYS:HB2  | 1:170:A:LYS:HE2  | 12       | 0.56          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD11 | 14       | 0.56          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD12 | 14       | 0.56          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD13 | 14       | 0.56          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 12       | 0.56          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 12       | 0.56          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 12       | 0.56          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 13       | 0.56          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 13       | 0.56          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 13       | 0.56          |
| (1,90)   | 1:124:A:GLY:H    | 1:92:A:VAL:HG11  | 3        | 0.56          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 13       | 0.56          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 13       | 0.56          |
| (1,43)   | 1:141:A:GLN:H    | 1:141:A:GLN:HG3  | 11       | 0.56          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG23  | 5        | 0.56          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 6        | 0.55          |
| (1,2014) | 1:77:A:ILE:HD11  | 1:126:A:VAL:HB   | 16       | 0.55          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE3  | 17       | 0.55          |
| (1,1843) | 1:147:A:ILE:HD13 | 1:102:A:VAL:HB   | 12       | 0.55          |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 5        | 0.55          |
| (1,1807) | 1:154:A:THR:HG22 | 1:155:A:GLY:H    | 3        | 0.55          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD11  | 1        | 0.55          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD12  | 1        | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD13  | 1        | 0.55          |
| (1,1645) | 1:108:A:ILE:HG23 | 1:84:A:PRO:HD2   | 15       | 0.55          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 7        | 0.55          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 7        | 0.55          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 7        | 0.55          |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 15       | 0.55          |
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE3  | 3        | 0.55          |
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE2  | 17       | 0.55          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 9        | 0.55          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 9        | 0.55          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 9        | 0.55          |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE3  | 15       | 0.55          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 14       | 0.55          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 14       | 0.55          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 14       | 0.55          |
| (1,1395) | 1:153:A:VAL:HG12 | 1:150:A:HIS:HA   | 4        | 0.55          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 8        | 0.55          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 14       | 0.55          |
| (1,363)  | 1:155:A:GLY:H    | 1:154:A:THR:HG22 | 3        | 0.55          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG23  | 10       | 0.55          |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG12 | 8        | 0.55          |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG21 | 11       | 0.55          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 11       | 0.55          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 16       | 0.55          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 14       | 0.55          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 7        | 0.55          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HG3   | 19       | 0.55          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 14       | 0.55          |
| (1,2025) | 1:144:A:LYS:HE2  | 1:143:A:TRP:HZ3  | 12       | 0.54          |
| (1,1956) | 1:69:A:LEU:HD12  | 1:150:A:HIS:HB3  | 3        | 0.54          |
| (1,1953) | 1:130:A:ILE:HG22 | 1:88:A:GLY:HA2   | 10       | 0.54          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE3  | 12       | 0.54          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 16       | 0.54          |
| (1,1722) | 1:69:A:LEU:HD22  | 1:150:A:HIS:HE1  | 9        | 0.54          |
| (1,1668) | 1:172:A:THR:HG23 | 1:172:A:THR:H    | 20       | 0.54          |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD21  | 16       | 0.54          |
| (1,1550) | 1:72:A:THR:HG23  | 1:69:A:LEU:HD12  | 19       | 0.54          |
| (1,1519) | 1:131:A:VAL:HG22 | 1:89:A:VAL:HG13  | 7        | 0.54          |
| (1,1510) | 1:115:A:HIS:HB3  | 1:116:A:LEU:HD22 | 8        | 0.54          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD21  | 7        | 0.54          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG12 | 15       | 0.54          |
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE2  | 9        | 0.54          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1442) | 1:73:A:GLU:HB2  | 1:74:A:LEU:HD11  | 19       | 0.54          |
| (1,1442) | 1:73:A:GLU:HB2  | 1:74:A:LEU:HD12  | 19       | 0.54          |
| (1,1442) | 1:73:A:GLU:HB2  | 1:74:A:LEU:HD13  | 19       | 0.54          |
| (1,1426) | 1:144:A:LYS:HB2 | 1:144:A:LYS:HE2  | 7        | 0.54          |
| (1,1426) | 1:144:A:LYS:HB2 | 1:144:A:LYS:HE2  | 17       | 0.54          |
| (1,1382) | 1:170:A:LYS:HB2 | 1:170:A:LYS:HE2  | 17       | 0.54          |
| (1,1319) | 1:90:A:TYR:H    | 1:90:A:TYR:HD1   | 12       | 0.54          |
| (1,263)  | 1:146:A:TRP:HE1 | 1:68:A:SER:HB3   | 13       | 0.54          |
| (1,199)  | 1:81:A:ASP:H    | 1:83:A:ILE:HD13  | 15       | 0.54          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG11 | 5        | 0.54          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG12 | 5        | 0.54          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG13 | 5        | 0.54          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG11 | 17       | 0.54          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG12 | 17       | 0.54          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG13 | 17       | 0.54          |
| (1,88)   | 1:90:A:TYR:H    | 1:104:A:ILE:HG22 | 12       | 0.54          |
| (1,25)   | 1:135:A:ASP:H   | 1:134:A:PRO:HG2  | 12       | 0.54          |
| (1,5)    | 1:107:A:ASN:H   | 1:107:A:ASN:HD22 | 8        | 0.54          |
| (1,2812) | 1:90:A:TYR:HD2  | 1:104:A:ILE:HG21 | 3        | 0.53          |
| (1,1911) | 1:85:A:SER:HB3  | 1:83:A:ILE:HG21  | 1        | 0.53          |
| (1,1804) | 1:123:A:CYS:HB3 | 1:95:A:LYS:HE2   | 14       | 0.53          |
| (1,1679) | 1:74:A:LEU:HD21 | 1:76:A:PRO:HG3   | 20       | 0.53          |
| (1,1550) | 1:72:A:THR:HG23 | 1:74:A:LEU:HD22  | 15       | 0.53          |
| (1,1502) | 1:84:A:PRO:HG2  | 1:75:A:LEU:HD22  | 2        | 0.53          |
| (1,1471) | 1:117:A:LYS:HG2 | 1:112:A:VAL:HG13 | 13       | 0.53          |
| (1,1442) | 1:73:A:GLU:HB2  | 1:74:A:LEU:HD11  | 14       | 0.53          |
| (1,1442) | 1:73:A:GLU:HB2  | 1:74:A:LEU:HD12  | 14       | 0.53          |
| (1,1442) | 1:73:A:GLU:HB2  | 1:74:A:LEU:HD13  | 14       | 0.53          |
| (1,1426) | 1:144:A:LYS:HB2 | 1:144:A:LYS:HE2  | 6        | 0.53          |
| (1,1426) | 1:144:A:LYS:HB2 | 1:144:A:LYS:HE3  | 9        | 0.53          |
| (1,1426) | 1:144:A:LYS:HB2 | 1:144:A:LYS:HE2  | 11       | 0.53          |
| (1,1426) | 1:144:A:LYS:HB2 | 1:144:A:LYS:HE3  | 13       | 0.53          |
| (1,1400) | 1:99:A:LEU:HD13 | 1:98:A:GLU:HB3   | 10       | 0.53          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG11 | 18       | 0.53          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG12 | 18       | 0.53          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG13 | 18       | 0.53          |
| (1,363)  | 1:155:A:GLY:H   | 1:153:A:VAL:HG22 | 8        | 0.53          |
| (1,202)  | 1:156:A:LYS:H   | 1:156:A:LYS:HG3  | 12       | 0.53          |
| (1,171)  | 1:129:A:GLY:H   | 1:89:A:VAL:HG21  | 20       | 0.53          |
| (1,171)  | 1:129:A:GLY:H   | 1:89:A:VAL:HG22  | 20       | 0.53          |
| (1,171)  | 1:129:A:GLY:H   | 1:89:A:VAL:HG23  | 20       | 0.53          |
| (1,135)  | 1:116:A:LEU:H   | 1:92:A:VAL:HG21  | 15       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 15       | 0.53          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 15       | 0.53          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG21  | 6        | 0.53          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 4        | 0.53          |
| (1,73)   | 1:125:A:SER:H    | 1:95:A:LYS:HG3   | 7        | 0.53          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 17       | 0.53          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 5        | 0.53          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG23 | 18       | 0.53          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HG3   | 9        | 0.53          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 6        | 0.53          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 11       | 0.53          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD11  | 15       | 0.53          |
| (1,2826) | 1:143:A:TRP:HZ2  | 1:147:A:ILE:HD12 | 13       | 0.52          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG22 | 14       | 0.52          |
| (1,2789) | 1:90:A:TYR:HD1   | 1:102:A:VAL:HB   | 7        | 0.52          |
| (1,2025) | 1:144:A:LYS:HE2  | 1:143:A:TRP:HZ3  | 2        | 0.52          |
| (1,2014) | 1:77:A:ILE:HD12  | 1:126:A:VAL:HB   | 19       | 0.52          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG22  | 5        | 0.52          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 2        | 0.52          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE2   | 15       | 0.52          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 8        | 0.52          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 8        | 0.52          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 8        | 0.52          |
| (1,1688) | 1:116:A:LEU:HD21 | 1:93:A:TYR:H     | 9        | 0.52          |
| (1,1550) | 1:72:A:THR:HG21  | 1:74:A:LEU:HD23  | 13       | 0.52          |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 3        | 0.52          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD13  | 15       | 0.52          |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 14       | 0.52          |
| (1,1494) | 1:172:A:THR:HB   | 1:171:A:VAL:HG12 | 11       | 0.52          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 11       | 0.52          |
| (1,1433) | 1:117:A:LYS:HD3  | 1:116:A:LEU:HD21 | 10       | 0.52          |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE3  | 3        | 0.52          |
| (1,1376) | 1:162:A:LYS:HD2  | 1:157:A:VAL:HG13 | 8        | 0.52          |
| (1,535)  | 1:125:A:SER:H    | 1:93:A:TYR:HD1   | 6        | 0.52          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 6        | 0.52          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG21 | 1        | 0.52          |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG13 | 17       | 0.52          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 3        | 0.52          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 15       | 0.52          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG2  | 7        | 0.52          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD22 | 2        | 0.52          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 13       | 0.52          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 19       | 0.52          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 4        | 0.52          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 12       | 0.52          |
| (1,5)    | 1:107:A:ASN:H    | 1:90:A:TYR:HE2   | 13       | 0.52          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD13  | 6        | 0.52          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 6        | 0.51          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG21 | 7        | 0.51          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 3        | 0.51          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 12       | 0.51          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HB   | 13       | 0.51          |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 13       | 0.51          |
| (1,1956) | 1:69:A:LEU:HD11  | 1:150:A:HIS:HB3  | 16       | 0.51          |
| (1,1947) | 1:70:A:THR:HB    | 1:67:A:LYS:HB2   | 9        | 0.51          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG22  | 8        | 0.51          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG21  | 9        | 0.51          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 17       | 0.51          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 19       | 0.51          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 20       | 0.51          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 20       | 0.51          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 1        | 0.51          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 1        | 0.51          |
| (1,1840) | 1:86:A:ALA:HB1   | 1:88:A:GLY:H     | 15       | 0.51          |
| (1,1807) | 1:154:A:THR:HG22 | 1:155:A:GLY:H    | 7        | 0.51          |
| (1,1807) | 1:154:A:THR:HG22 | 1:155:A:GLY:H    | 11       | 0.51          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE2   | 17       | 0.51          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 6        | 0.51          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 6        | 0.51          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 6        | 0.51          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 15       | 0.51          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 15       | 0.51          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 15       | 0.51          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 20       | 0.51          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 20       | 0.51          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 20       | 0.51          |
| (1,1506) | 1:170:A:LYS:HE2  | 1:171:A:VAL:H    | 9        | 0.51          |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 4        | 0.51          |
| (1,1497) | 1:130:A:ILE:HG22 | 1:131:A:VAL:H    | 16       | 0.51          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 7        | 0.51          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 7        | 0.51          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 7        | 0.51          |
| (1,1432) | 1:95:A:LYS:HD3   | 1:123:A:CYS:H    | 4        | 0.51          |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE3  | 20       | 0.51          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 19       | 0.51          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 19       | 0.51          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 19       | 0.51          |
| (1,1395) | 1:153:A:VAL:HG12 | 1:150:A:HIS:HA   | 8        | 0.51          |
| (1,1395) | 1:153:A:VAL:HG13 | 1:150:A:HIS:HA   | 20       | 0.51          |
| (1,363)  | 1:155:A:GLY:H    | 1:154:A:THR:HG22 | 7        | 0.51          |
| (1,363)  | 1:155:A:GLY:H    | 1:154:A:THR:HG22 | 11       | 0.51          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG22 | 6        | 0.51          |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG2  | 2        | 0.51          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG11 | 20       | 0.51          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG12 | 20       | 0.51          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG13 | 20       | 0.51          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 2        | 0.51          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 2        | 0.51          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG3  | 12       | 0.51          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 16       | 0.51          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG23 | 19       | 0.51          |
| (1,25)   | 1:135:A:ASP:H    | 1:134:A:PRO:HG2  | 3        | 0.51          |
| (1,25)   | 1:135:A:ASP:H    | 1:134:A:PRO:HG2  | 11       | 0.51          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 16       | 0.51          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 18       | 0.51          |
| (1,1861) | 1:104:A:ILE:HD11 | 1:140:A:THR:H    | 2        | 0.5           |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 2        | 0.5           |
| (1,1629) | 1:77:A:ILE:HG21  | 1:120:A:PRO:HA   | 2        | 0.5           |
| (1,1566) | 1:119:A:VAL:HG22 | 1:167:A:THR:HG23 | 14       | 0.5           |
| (1,1557) | 1:147:A:ILE:HD12 | 1:144:A:LYS:HE2  | 12       | 0.5           |
| (1,1528) | 1:148:A:GLU:HG2  | 1:157:A:VAL:HG21 | 10       | 0.5           |
| (1,1497) | 1:130:A:ILE:HG21 | 1:131:A:VAL:H    | 18       | 0.5           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 3        | 0.5           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 3        | 0.5           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 3        | 0.5           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 5        | 0.5           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 5        | 0.5           |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 5        | 0.5           |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG12  | 17       | 0.5           |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE2  | 18       | 0.5           |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 20       | 0.5           |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 20       | 0.5           |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 20       | 0.5           |
| (1,1395) | 1:153:A:VAL:HG11 | 1:150:A:HIS:HA   | 15       | 0.5           |
| (1,1382) | 1:170:A:LYS:HB2  | 1:170:A:LYS:HE3  | 18       | 0.5           |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 3        | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG23 | 17       | 0.5           |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG21  | 19       | 0.5           |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG22  | 19       | 0.5           |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG23  | 19       | 0.5           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG11 | 11       | 0.5           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG12 | 11       | 0.5           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG13 | 11       | 0.5           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 18       | 0.5           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 18       | 0.5           |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 18       | 0.5           |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD11 | 5        | 0.5           |
| (1,90)   | 1:124:A:GLY:H    | 1:92:A:VAL:HG11  | 2        | 0.5           |
| (1,73)   | 1:125:A:SER:H    | 1:95:A:LYS:HG3   | 5        | 0.5           |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG3  | 17       | 0.5           |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 5        | 0.5           |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 14       | 0.5           |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HG3   | 14       | 0.5           |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 1        | 0.5           |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 1        | 0.5           |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 4        | 0.5           |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD11  | 5        | 0.5           |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 9        | 0.5           |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD13  | 17       | 0.5           |
| (1,1947) | 1:70:A:THR:HB    | 1:67:A:LYS:HB2   | 20       | 0.49          |
| (1,1877) | 1:112:A:VAL:HA   | 1:90:A:TYR:HB2   | 7        | 0.49          |
| (1,1861) | 1:104:A:ILE:HD12 | 1:140:A:THR:H    | 16       | 0.49          |
| (1,1843) | 1:147:A:ILE:HD13 | 1:102:A:VAL:HB   | 14       | 0.49          |
| (1,1840) | 1:86:A:ALA:HB1   | 1:88:A:GLY:H     | 4        | 0.49          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 4        | 0.49          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 4        | 0.49          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 4        | 0.49          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD11  | 3        | 0.49          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD12  | 3        | 0.49          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD13  | 3        | 0.49          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 19       | 0.49          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 19       | 0.49          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 19       | 0.49          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 14       | 0.49          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 14       | 0.49          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 14       | 0.49          |
| (1,1497) | 1:130:A:ILE:HG21 | 1:131:A:VAL:H    | 5        | 0.49          |
| (1,1497) | 1:130:A:ILE:HG22 | 1:131:A:VAL:H    | 6        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 17       | 0.49          |
| (1,1494) | 1:172:A:THR:HB   | 1:173:A:LEU:HD12 | 6        | 0.49          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 1        | 0.49          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 1        | 0.49          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 1        | 0.49          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD11  | 8        | 0.49          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD12  | 8        | 0.49          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD13  | 8        | 0.49          |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD3  | 3        | 0.49          |
| (1,311)  | 1:88:A:GLY:H     | 1:106:A:ARG:HD2  | 19       | 0.49          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD11 | 10       | 0.49          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD11 | 11       | 0.49          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD12 | 11       | 0.49          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD13 | 11       | 0.49          |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG21  | 11       | 0.49          |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG22  | 11       | 0.49          |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG23  | 11       | 0.49          |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD13 | 17       | 0.49          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 20       | 0.49          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 9        | 0.49          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 5        | 0.49          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD13  | 2        | 0.49          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD11  | 3        | 0.49          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD11  | 10       | 0.49          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD11  | 12       | 0.49          |
| (1,2799) | 1:93:A:TYR:HE2   | 1:69:A:LEU:HD13  | 2        | 0.48          |
| (1,1843) | 1:147:A:ILE:HD11 | 1:102:A:VAL:HB   | 5        | 0.48          |
| (1,1840) | 1:86:A:ALA:HB1   | 1:88:A:GLY:H     | 8        | 0.48          |
| (1,1840) | 1:86:A:ALA:HB2   | 1:88:A:GLY:H     | 12       | 0.48          |
| (1,1726) | 1:69:A:LEU:HD12  | 1:150:A:HIS:H    | 4        | 0.48          |
| (1,1629) | 1:77:A:ILE:HG21  | 1:120:A:PRO:HA   | 3        | 0.48          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 18       | 0.48          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 18       | 0.48          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 18       | 0.48          |
| (1,1592) | 1:141:A:GLN:HG3  | 1:142:A:ALA:HB3  | 8        | 0.48          |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 10       | 0.48          |
| (1,1497) | 1:130:A:ILE:HG21 | 1:131:A:VAL:H    | 8        | 0.48          |
| (1,1494) | 1:172:A:THR:HB   | 1:171:A:VAL:HG12 | 20       | 0.48          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 15       | 0.48          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 15       | 0.48          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 15       | 0.48          |
| (1,1422) | 1:145:A:LEU:HD22 | 1:145:A:LEU:H    | 15       | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 7        | 0.48          |
| (1,1396) | 1:83:A:ILE:HG22  | 1:90:A:TYR:HD2   | 1        | 0.48          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 17       | 0.48          |
| (1,236)  | 1:156:A:LYS:H    | 1:156:A:LYS:HE2  | 5        | 0.48          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 4        | 0.48          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 15       | 0.48          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD11 | 16       | 0.48          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD12 | 16       | 0.48          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD13 | 16       | 0.48          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG22 | 9        | 0.48          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 12       | 0.48          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 10       | 0.48          |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD13 | 10       | 0.48          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 4        | 0.48          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 1        | 0.48          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 18       | 0.48          |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG22  | 13       | 0.48          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 2        | 0.48          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 8        | 0.48          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD21 | 4        | 0.48          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD11  | 16       | 0.48          |
| (1,2869) | 1:115:A:HIS:HE1  | 1:112:A:VAL:HG13 | 10       | 0.47          |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 4        | 0.47          |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 7        | 0.47          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 15       | 0.47          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 18       | 0.47          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 18       | 0.47          |
| (1,1861) | 1:104:A:ILE:HD12 | 1:140:A:THR:H    | 13       | 0.47          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE2   | 10       | 0.47          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE2   | 16       | 0.47          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 2        | 0.47          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 2        | 0.47          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 2        | 0.47          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 7        | 0.47          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 7        | 0.47          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 7        | 0.47          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 8        | 0.47          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 8        | 0.47          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 8        | 0.47          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 12       | 0.47          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 12       | 0.47          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 12       | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1566) | 1:119:A:VAL:HG23 | 1:167:A:THR:HG22 | 9        | 0.47          |
| (1,1514) | 1:147:A:ILE:HD13 | 1:157:A:VAL:H    | 7        | 0.47          |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 7        | 0.47          |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 20       | 0.47          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 13       | 0.47          |
| (1,1469) | 1:156:A:LYS:HG3  | 1:98:A:GLU:HG2   | 2        | 0.47          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 17       | 0.47          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 17       | 0.47          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 17       | 0.47          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD11  | 15       | 0.47          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD12  | 15       | 0.47          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD13  | 15       | 0.47          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 5        | 0.47          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 5        | 0.47          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 5        | 0.47          |
| (1,1396) | 1:83:A:ILE:HG22  | 1:90:A:TYR:HD2   | 16       | 0.47          |
| (1,1383) | 1:80:A:ALA:HB3   | 1:83:A:ILE:HG13  | 2        | 0.47          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 4        | 0.47          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 12       | 0.47          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 4        | 0.47          |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG2  | 3        | 0.47          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG3  | 9        | 0.47          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD12  | 6        | 0.47          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD13  | 12       | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 1        | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 1        | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 1        | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 2        | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 2        | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 2        | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 6        | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 6        | 0.47          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 6        | 0.47          |
| (1,111)  | 1:148:A:GLU:H    | 1:148:A:GLU:HG3  | 14       | 0.47          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 7        | 0.47          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD23 | 3        | 0.47          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD23 | 13       | 0.47          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 11       | 0.47          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 9        | 0.47          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG23 | 6        | 0.46          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:153:A:VAL:HG21 | 8        | 0.46          |
| (1,2799) | 1:93:A:TYR:HE1   | 1:69:A:LEU:HD12  | 16       | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 14       | 0.46          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 4        | 0.46          |
| (1,1878) | 1:147:A:ILE:HG22 | 1:148:A:GLU:HB2  | 6        | 0.46          |
| (1,1861) | 1:104:A:ILE:HD12 | 1:140:A:THR:H    | 9        | 0.46          |
| (1,1840) | 1:86:A:ALA:HB2   | 1:88:A:GLY:H     | 6        | 0.46          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE2   | 8        | 0.46          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 17       | 0.46          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 17       | 0.46          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 17       | 0.46          |
| (1,1702) | 1:99:A:LEU:HD23  | 1:93:A:TYR:HA    | 8        | 0.46          |
| (1,1679) | 1:74:A:LEU:HD22  | 1:76:A:PRO:HG3   | 13       | 0.46          |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 8        | 0.46          |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 9        | 0.46          |
| (1,1551) | 1:99:A:LEU:HD23  | 1:103:A:GLY:H    | 19       | 0.46          |
| (1,1500) | 1:151:A:ILE:HG21 | 1:152:A:LYS:HE3  | 12       | 0.46          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 7        | 0.46          |
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE3  | 18       | 0.46          |
| (1,1448) | 1:156:A:LYS:HD3  | 1:156:A:LYS:H    | 18       | 0.46          |
| (1,1409) | 1:73:A:GLU:HG2   | 1:74:A:LEU:HD21  | 11       | 0.46          |
| (1,1409) | 1:73:A:GLU:HG2   | 1:74:A:LEU:HD22  | 11       | 0.46          |
| (1,1409) | 1:73:A:GLU:HG2   | 1:74:A:LEU:HD23  | 11       | 0.46          |
| (1,1399) | 1:138:A:VAL:HG23 | 1:137:A:ALA:H    | 17       | 0.46          |
| (1,1319) | 1:90:A:TYR:H     | 1:90:A:TYR:HD1   | 7        | 0.46          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 9        | 0.46          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 9        | 0.46          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 9        | 0.46          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 3        | 0.46          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 7        | 0.46          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG22 | 7        | 0.46          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG23 | 20       | 0.46          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 13       | 0.46          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 13       | 0.46          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 13       | 0.46          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 18       | 0.46          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 18       | 0.46          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 18       | 0.46          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG21 | 5        | 0.46          |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD11 | 5        | 0.46          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG21 | 4        | 0.45          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG22  | 7        | 0.45          |
| (1,1843) | 1:147:A:ILE:HD11 | 1:102:A:VAL:HB   | 1        | 0.45          |
| (1,1702) | 1:99:A:LEU:HD23  | 1:93:A:TYR:HA    | 13       | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 13       | 0.45          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 13       | 0.45          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 13       | 0.45          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 20       | 0.45          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 20       | 0.45          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 20       | 0.45          |
| (1,1550) | 1:72:A:THR:HG22  | 1:69:A:LEU:HD13  | 18       | 0.45          |
| (1,1506) | 1:156:A:LYS:HE3  | 1:157:A:VAL:H    | 4        | 0.45          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 6        | 0.45          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 14       | 0.45          |
| (1,1422) | 1:145:A:LEU:HD21 | 1:145:A:LEU:H    | 13       | 0.45          |
| (1,1402) | 1:112:A:VAL:HA   | 1:115:A:HIS:HD2  | 6        | 0.45          |
| (1,1396) | 1:83:A:ILE:HG21  | 1:90:A:TYR:HD2   | 2        | 0.45          |
| (1,1395) | 1:153:A:VAL:HG11 | 1:150:A:HIS:HA   | 17       | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 2        | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 2        | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 2        | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 5        | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 5        | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 5        | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 7        | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 7        | 0.45          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 7        | 0.45          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 11       | 0.45          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG21 | 15       | 0.45          |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD13  | 18       | 0.45          |
| (1,210)  | 1:116:A:LEU:H    | 1:112:A:VAL:HA   | 5        | 0.45          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 20       | 0.45          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG11 | 15       | 0.45          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG12 | 15       | 0.45          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG13 | 15       | 0.45          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 16       | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 3        | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 3        | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 3        | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 4        | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 4        | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 4        | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 14       | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 14       | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 14       | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 19       | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 19       | 0.45          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 19       | 0.45          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 9        | 0.45          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 6        | 0.45          |
| (1,25)   | 1:135:A:ASP:H    | 1:134:A:PRO:HB2  | 4        | 0.45          |
| (1,25)   | 1:135:A:ASP:H    | 1:134:A:PRO:HG2  | 8        | 0.45          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 8        | 0.44          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 10       | 0.44          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 4        | 0.44          |
| (1,1878) | 1:147:A:ILE:HG23 | 1:148:A:GLU:HB2  | 11       | 0.44          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 14       | 0.44          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 10       | 0.44          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 10       | 0.44          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 10       | 0.44          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 14       | 0.44          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 14       | 0.44          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 14       | 0.44          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 18       | 0.44          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 18       | 0.44          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 18       | 0.44          |
| (1,1645) | 1:108:A:ILE:HG22 | 1:84:A:PRO:HD2   | 18       | 0.44          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 5        | 0.44          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 5        | 0.44          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 5        | 0.44          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 16       | 0.44          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 16       | 0.44          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 16       | 0.44          |
| (1,1497) | 1:130:A:ILE:HG22 | 1:131:A:VAL:H    | 10       | 0.44          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 18       | 0.44          |
| (1,1433) | 1:170:A:LYS:HD2  | 1:167:A:THR:HG21 | 4        | 0.44          |
| (1,1422) | 1:145:A:LEU:HD21 | 1:145:A:LEU:H    | 7        | 0.44          |
| (1,1422) | 1:145:A:LEU:HD21 | 1:145:A:LEU:H    | 20       | 0.44          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 13       | 0.44          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 13       | 0.44          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 13       | 0.44          |
| (1,1377) | 1:89:A:VAL:HG23  | 1:131:A:VAL:HG11 | 5        | 0.44          |
| (1,1377) | 1:89:A:VAL:HG23  | 1:139:A:LEU:HD21 | 13       | 0.44          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG23 | 3        | 0.44          |
| (1,324)  | 1:154:A:THR:H    | 1:156:A:LYS:HG2  | 11       | 0.44          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 12       | 0.44          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 7        | 0.44          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 9        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 11       | 0.44          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 14       | 0.44          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 20       | 0.44          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 20       | 0.44          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 20       | 0.44          |
| (1,101)  | 1:89:A:VAL:H     | 1:139:A:LEU:HD21 | 11       | 0.44          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG23 | 19       | 0.44          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 20       | 0.44          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 18       | 0.44          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 17       | 0.44          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 7        | 0.44          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG23 | 10       | 0.43          |
| (1,2799) | 1:93:A:TYR:HE1   | 1:74:A:LEU:HD22  | 9        | 0.43          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB1   | 10       | 0.43          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 1        | 0.43          |
| (1,2789) | 1:90:A:TYR:HD1   | 1:102:A:VAL:HB   | 17       | 0.43          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 19       | 0.43          |
| (1,2014) | 1:77:A:ILE:HD12  | 1:126:A:VAL:HB   | 11       | 0.43          |
| (1,2014) | 1:77:A:ILE:HD12  | 1:126:A:VAL:HB   | 14       | 0.43          |
| (1,2013) | 1:98:A:GLU:HG2   | 1:98:A:GLU:H     | 6        | 0.43          |
| (1,1947) | 1:70:A:THR:HB    | 1:67:A:LYS:HB2   | 19       | 0.43          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG21  | 4        | 0.43          |
| (1,1861) | 1:104:A:ILE:HD13 | 1:140:A:THR:H    | 18       | 0.43          |
| (1,1843) | 1:147:A:ILE:HD12 | 1:102:A:VAL:HB   | 2        | 0.43          |
| (1,1840) | 1:86:A:ALA:HB1   | 1:88:A:GLY:H     | 16       | 0.43          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 3        | 0.43          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 3        | 0.43          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 3        | 0.43          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 5        | 0.43          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 5        | 0.43          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 5        | 0.43          |
| (1,1690) | 1:145:A:LEU:HD21 | 1:67:A:LYS:H     | 1        | 0.43          |
| (1,1690) | 1:145:A:LEU:HD22 | 1:67:A:LYS:H     | 1        | 0.43          |
| (1,1690) | 1:145:A:LEU:HD23 | 1:67:A:LYS:H     | 1        | 0.43          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 9        | 0.43          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 9        | 0.43          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 9        | 0.43          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD21 | 20       | 0.43          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD22 | 20       | 0.43          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD23 | 20       | 0.43          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HD12 | 2        | 0.43          |
| (1,1510) | 1:115:A:HIS:HB3  | 1:116:A:LEU:HD22 | 13       | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1420) | 1:87:A:SER:HB3   | 1:106:A:ARG:HB2  | 20       | 0.43          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 6        | 0.43          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 6        | 0.43          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 6        | 0.43          |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 15       | 0.43          |
| (1,1395) | 1:153:A:VAL:HG11 | 1:150:A:HIS:HA   | 1        | 0.43          |
| (1,1395) | 1:153:A:VAL:HG12 | 1:150:A:HIS:HA   | 12       | 0.43          |
| (1,394)  | 1:121:A:GLU:H    | 1:116:A:LEU:HD22 | 18       | 0.43          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG21 | 1        | 0.43          |
| (1,324)  | 1:154:A:THR:H    | 1:156:A:LYS:HG2  | 12       | 0.43          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD21 | 1        | 0.43          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD22 | 1        | 0.43          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD23 | 1        | 0.43          |
| (1,236)  | 1:156:A:LYS:H    | 1:156:A:LYS:HE2  | 15       | 0.43          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 14       | 0.43          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 11       | 0.43          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 4        | 0.43          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD13  | 5        | 0.43          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 14       | 0.43          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD11 | 9        | 0.43          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 16       | 0.43          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 16       | 0.43          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 16       | 0.43          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 1        | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 5        | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 5        | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 5        | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 9        | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 9        | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 9        | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 10       | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 10       | 0.43          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 10       | 0.43          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD22 | 6        | 0.43          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 10       | 0.43          |
| (1,9)    | 1:79:A:GLU:H     | 1:77:A:ILE:HA    | 1        | 0.43          |
| (1,5)    | 1:107:A:ASN:H    | 1:90:A:TYR:HE2   | 12       | 0.43          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 8        | 0.43          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD11  | 19       | 0.43          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG21 | 7        | 0.42          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:153:A:VAL:HG21 | 17       | 0.42          |
| (1,2791) | 1:90:A:TYR:HE1   | 1:112:A:VAL:HG22 | 7        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 4        | 0.42          |
| (1,1878) | 1:147:A:ILE:HG22 | 1:148:A:GLU:HB2  | 2        | 0.42          |
| (1,1878) | 1:147:A:ILE:HG23 | 1:148:A:GLU:HB2  | 5        | 0.42          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 13       | 0.42          |
| (1,1861) | 1:104:A:ILE:HD13 | 1:140:A:THR:H    | 1        | 0.42          |
| (1,1856) | 1:87:A:SER:HB3   | 1:106:A:ARG:HD3  | 19       | 0.42          |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 10       | 0.42          |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 17       | 0.42          |
| (1,1812) | 1:76:A:PRO:HG3   | 1:74:A:LEU:HB3   | 18       | 0.42          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 19       | 0.42          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 19       | 0.42          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 19       | 0.42          |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 4        | 0.42          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 1        | 0.42          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 7        | 0.42          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 7        | 0.42          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 7        | 0.42          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 17       | 0.42          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 17       | 0.42          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 17       | 0.42          |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG23 | 2        | 0.42          |
| (1,1551) | 1:99:A:LEU:HD23  | 1:103:A:GLY:H    | 2        | 0.42          |
| (1,1550) | 1:72:A:THR:HG21  | 1:69:A:LEU:HD11  | 20       | 0.42          |
| (1,1506) | 1:156:A:LYS:HE3  | 1:157:A:VAL:H    | 7        | 0.42          |
| (1,1494) | 1:172:A:THR:HB   | 1:171:A:VAL:HG22 | 17       | 0.42          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 8        | 0.42          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 8        | 0.42          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 8        | 0.42          |
| (1,1422) | 1:145:A:LEU:HD21 | 1:145:A:LEU:H    | 4        | 0.42          |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 9        | 0.42          |
| (1,1390) | 1:152:A:LYS:HE3  | 1:148:A:GLU:HB3  | 8        | 0.42          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 1        | 0.42          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 1        | 0.42          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 1        | 0.42          |
| (1,231)  | 1:140:A:THR:H    | 1:136:A:LYS:HE2  | 11       | 0.42          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG3  | 2        | 0.42          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 10       | 0.42          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD13 | 6        | 0.42          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD13 | 7        | 0.42          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 1        | 0.42          |
| (1,159)  | 1:153:A:VAL:H    | 1:154:A:THR:HG22 | 5        | 0.42          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 19       | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 19       | 0.42          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 19       | 0.42          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 11       | 0.42          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 11       | 0.42          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 11       | 0.42          |
| (1,92)   | 1:95:A:LYS:H     | 1:77:A:ILE:HG22  | 19       | 0.42          |
| (1,83)   | 1:111:A:SER:H    | 1:83:A:ILE:HG23  | 3        | 0.42          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 7        | 0.42          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 15       | 0.42          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 18       | 0.42          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 1        | 0.42          |
| (1,24)   | 1:100:A:GLN:H    | 1:99:A:LEU:HB2   | 11       | 0.42          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 13       | 0.42          |
| (1,2869) | 1:115:A:HIS:HE1  | 1:116:A:LEU:HD21 | 17       | 0.41          |
| (1,2795) | 1:93:A:TYR:HD2   | 1:91:A:ALA:HB2   | 19       | 0.41          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 4        | 0.41          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD11 | 13       | 0.41          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD12 | 13       | 0.41          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD13 | 13       | 0.41          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 16       | 0.41          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 16       | 0.41          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 16       | 0.41          |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 2        | 0.41          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 5        | 0.41          |
| (1,1665) | 1:140:A:THR:HG21 | 1:141:A:GLN:H    | 14       | 0.41          |
| (1,1550) | 1:72:A:THR:HG22  | 1:69:A:LEU:HD11  | 17       | 0.41          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG12 | 7        | 0.41          |
| (1,1402) | 1:112:A:VAL:HA   | 1:90:A:TYR:HE1   | 12       | 0.41          |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 1        | 0.41          |
| (1,1388) | 1:95:A:LYS:HD2   | 1:77:A:ILE:HD13  | 14       | 0.41          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 14       | 0.41          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 14       | 0.41          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 14       | 0.41          |
| (1,231)  | 1:140:A:THR:H    | 1:136:A:LYS:HE2  | 8        | 0.41          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG3  | 19       | 0.41          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 4        | 0.41          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 19       | 0.41          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD13  | 16       | 0.41          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD13 | 1        | 0.41          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 5        | 0.41          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG21 | 14       | 0.41          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 2        | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 2        | 0.41          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 2        | 0.41          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 12       | 0.41          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 12       | 0.41          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 12       | 0.41          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 19       | 0.41          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 20       | 0.41          |
| (1,101)  | 1:89:A:VAL:H     | 1:139:A:LEU:HD21 | 1        | 0.41          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD21 | 14       | 0.41          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG21 | 10       | 0.41          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 2        | 0.41          |
| (1,5)    | 1:107:A:ASN:H    | 1:90:A:TYR:HE2   | 11       | 0.41          |
| (1,5)    | 1:107:A:ASN:H    | 1:90:A:TYR:HE2   | 14       | 0.41          |
| (1,1)    | 1:83:A:ILE:H     | 1:83:A:ILE:HD12  | 20       | 0.41          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG22 | 12       | 0.4           |
| (1,1999) | 1:98:A:GLU:HG3   | 1:100:A:GLN:HE22 | 16       | 0.4           |
| (1,1963) | 1:154:A:THR:HB   | 1:156:A:LYS:HE2  | 5        | 0.4           |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 2        | 0.4           |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG22  | 18       | 0.4           |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 9        | 0.4           |
| (1,1859) | 1:77:A:ILE:HD13  | 1:76:A:PRO:HB2   | 10       | 0.4           |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 1        | 0.4           |
| (1,1665) | 1:140:A:THR:HG21 | 1:141:A:GLN:H    | 2        | 0.4           |
| (1,1665) | 1:140:A:THR:HG21 | 1:141:A:GLN:H    | 10       | 0.4           |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HB3  | 2        | 0.4           |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 3        | 0.4           |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 3        | 0.4           |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 3        | 0.4           |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG22 | 13       | 0.4           |
| (1,1510) | 1:115:A:HIS:HB3  | 1:167:A:THR:HG21 | 19       | 0.4           |
| (1,1448) | 1:156:A:LYS:HD2  | 1:156:A:LYS:H    | 1        | 0.4           |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 12       | 0.4           |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 12       | 0.4           |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 12       | 0.4           |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 5        | 0.4           |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 16       | 0.4           |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 4        | 0.4           |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 4        | 0.4           |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 4        | 0.4           |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD23 | 1        | 0.4           |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 20       | 0.4           |
| (1,351)  | 1:100:A:GLN:HE22 | 1:98:A:GLU:HG3   | 16       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 16       | 0.4           |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD12 | 8        | 0.4           |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD12 | 11       | 0.4           |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG21  | 13       | 0.4           |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG22  | 13       | 0.4           |
| (1,171)  | 1:129:A:GLY:H    | 1:89:A:VAL:HG23  | 13       | 0.4           |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG21 | 2        | 0.4           |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG21 | 10       | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 7        | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 7        | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 7        | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 8        | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 8        | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 8        | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 16       | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 16       | 0.4           |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 16       | 0.4           |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 6        | 0.4           |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD12 | 20       | 0.4           |
| (1,73)   | 1:125:A:SER:H    | 1:95:A:LYS:HG3   | 18       | 0.4           |
| (1,71)   | 1:71:A:GLU:H     | 1:69:A:LEU:HG    | 12       | 0.4           |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG2  | 1        | 0.4           |
| (1,63)   | 1:170:A:LYS:H    | 1:166:A:ASN:HB2  | 7        | 0.4           |
| (1,39)   | 1:114:A:ALA:H    | 1:83:A:ILE:HG21  | 16       | 0.4           |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 5        | 0.39          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 3        | 0.39          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD22 | 6        | 0.39          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG21  | 14       | 0.39          |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 6        | 0.39          |
| (1,1702) | 1:99:A:LEU:HD23  | 1:93:A:TYR:HA    | 1        | 0.39          |
| (1,1702) | 1:99:A:LEU:HD21  | 1:93:A:TYR:HA    | 16       | 0.39          |
| (1,1688) | 1:116:A:LEU:HD22 | 1:93:A:TYR:H     | 7        | 0.39          |
| (1,1688) | 1:116:A:LEU:HD22 | 1:93:A:TYR:H     | 14       | 0.39          |
| (1,1688) | 1:116:A:LEU:HD21 | 1:93:A:TYR:H     | 16       | 0.39          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD11  | 8        | 0.39          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD12  | 8        | 0.39          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD13  | 8        | 0.39          |
| (1,1681) | 1:156:A:LYS:HG2  | 1:99:A:LEU:HD11  | 11       | 0.39          |
| (1,1681) | 1:156:A:LYS:HG2  | 1:99:A:LEU:HD12  | 11       | 0.39          |
| (1,1681) | 1:156:A:LYS:HG2  | 1:99:A:LEU:HD13  | 11       | 0.39          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 6        | 0.39          |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 6        | 0.39          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 6        | 0.39          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 6        | 0.39          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 6        | 0.39          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 9        | 0.39          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 9        | 0.39          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 9        | 0.39          |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG23 | 18       | 0.39          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 2        | 0.39          |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 9        | 0.39          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG11 | 3        | 0.39          |
| (1,1420) | 1:87:A:SER:HB3   | 1:106:A:ARG:HB2  | 10       | 0.39          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 16       | 0.39          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 16       | 0.39          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 16       | 0.39          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 3        | 0.39          |
| (1,231)  | 1:140:A:THR:H    | 1:136:A:LYS:HE2  | 18       | 0.39          |
| (1,210)  | 1:116:A:LEU:H    | 1:112:A:VAL:HA   | 3        | 0.39          |
| (1,210)  | 1:116:A:LEU:H    | 1:112:A:VAL:HA   | 6        | 0.39          |
| (1,210)  | 1:116:A:LEU:H    | 1:112:A:VAL:HA   | 7        | 0.39          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD12 | 3        | 0.39          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 6        | 0.39          |
| (1,159)  | 1:153:A:VAL:H    | 1:154:A:THR:HG22 | 10       | 0.39          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 17       | 0.39          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 17       | 0.39          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 17       | 0.39          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 4        | 0.39          |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD11 | 2        | 0.39          |
| (1,90)   | 1:124:A:GLY:H    | 1:77:A:ILE:HG13  | 13       | 0.39          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 12       | 0.39          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 1        | 0.39          |
| (1,73)   | 1:125:A:SER:H    | 1:77:A:ILE:HB    | 19       | 0.39          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD22 | 20       | 0.39          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 16       | 0.39          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 9        | 0.39          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD21 | 16       | 0.39          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 18       | 0.38          |
| (1,2014) | 1:77:A:ILE:HD11  | 1:126:A:VAL:HB   | 8        | 0.38          |
| (1,1999) | 1:98:A:GLU:HG3   | 1:100:A:GLN:HE22 | 1        | 0.38          |
| (1,1948) | 1:87:A:SER:HB3   | 1:131:A:VAL:H    | 13       | 0.38          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 19       | 0.38          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG22  | 3        | 0.38          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 16       | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1850) | 1:147:A:ILE:HD12 | 1:148:A:GLU:HG3  | 12       | 0.38          |
| (1,1702) | 1:99:A:LEU:HD22  | 1:93:A:TYR:HA    | 10       | 0.38          |
| (1,1665) | 1:140:A:THR:HG22 | 1:141:A:GLN:H    | 9        | 0.38          |
| (1,1665) | 1:140:A:THR:HG22 | 1:141:A:GLN:H    | 15       | 0.38          |
| (1,1659) | 1:104:A:ILE:HG22 | 1:143:A:TRP:HA   | 16       | 0.38          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 18       | 0.38          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 18       | 0.38          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 18       | 0.38          |
| (1,1565) | 1:167:A:THR:HA   | 1:168:A:PHE:HB2  | 15       | 0.38          |
| (1,1519) | 1:66:A:VAL:HG11  | 1:89:A:VAL:HG11  | 14       | 0.38          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 10       | 0.38          |
| (1,1485) | 1:85:A:SER:HB3   | 1:108:A:ILE:HB   | 12       | 0.38          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 4        | 0.38          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 4        | 0.38          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 4        | 0.38          |
| (1,1422) | 1:145:A:LEU:HD21 | 1:145:A:LEU:H    | 5        | 0.38          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 7        | 0.38          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 7        | 0.38          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 7        | 0.38          |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 13       | 0.38          |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 20       | 0.38          |
| (1,1388) | 1:95:A:LYS:HD2   | 1:77:A:ILE:HD13  | 12       | 0.38          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 10       | 0.38          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 10       | 0.38          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 10       | 0.38          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 16       | 0.38          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 16       | 0.38          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 16       | 0.38          |
| (1,351)  | 1:100:A:GLN:HE22 | 1:98:A:GLU:HG3   | 1        | 0.38          |
| (1,343)  | 1:96:A:SER:H     | 1:95:A:LYS:HD2   | 20       | 0.38          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 6        | 0.38          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 3        | 0.38          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 18       | 0.38          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 2        | 0.38          |
| (1,202)  | 1:156:A:LYS:H    | 1:156:A:LYS:HG3  | 11       | 0.38          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD12 | 17       | 0.38          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG22 | 9        | 0.38          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG22 | 15       | 0.38          |
| (1,149)  | 1:135:A:ASP:H    | 1:133:A:GLU:HG3  | 10       | 0.38          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG22 | 8        | 0.38          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 19       | 0.38          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 19       | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 19       | 0.38          |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG11 | 12       | 0.38          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD23 | 1        | 0.38          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD22 | 11       | 0.38          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD23 | 18       | 0.38          |
| (1,52)   | 1:113:A:SER:H    | 1:112:A:VAL:HG22 | 8        | 0.38          |
| (1,5)    | 1:107:A:ASN:H    | 1:90:A:TYR:HE2   | 4        | 0.38          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 19       | 0.38          |
| (1,1994) | 1:162:A:LYS:HE3  | 1:162:A:LYS:H    | 18       | 0.37          |
| (1,1984) | 1:69:A:LEU:HD12  | 1:151:A:ILE:H    | 15       | 0.37          |
| (1,1947) | 1:70:A:THR:HB    | 1:67:A:LYS:HB2   | 4        | 0.37          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 1        | 0.37          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 11       | 0.37          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 20       | 0.37          |
| (1,1877) | 1:112:A:VAL:HA   | 1:90:A:TYR:HB2   | 10       | 0.37          |
| (1,1877) | 1:112:A:VAL:HA   | 1:90:A:TYR:HB2   | 20       | 0.37          |
| (1,1861) | 1:104:A:ILE:HD12 | 1:140:A:THR:H    | 5        | 0.37          |
| (1,1861) | 1:104:A:ILE:HD11 | 1:140:A:THR:H    | 15       | 0.37          |
| (1,1850) | 1:147:A:ILE:HD13 | 1:148:A:GLU:HG3  | 20       | 0.37          |
| (1,1840) | 1:86:A:ALA:HB1   | 1:88:A:GLY:H     | 11       | 0.37          |
| (1,1840) | 1:86:A:ALA:HB2   | 1:88:A:GLY:H     | 14       | 0.37          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE3   | 19       | 0.37          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 1        | 0.37          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 1        | 0.37          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 1        | 0.37          |
| (1,1702) | 1:99:A:LEU:HD22  | 1:93:A:TYR:HA    | 7        | 0.37          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 4        | 0.37          |
| (1,1645) | 1:108:A:ILE:HG23 | 1:84:A:PRO:HD2   | 1        | 0.37          |
| (1,1584) | 1:95:A:LYS:HD2   | 1:124:A:GLY:H    | 14       | 0.37          |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG23 | 9        | 0.37          |
| (1,1551) | 1:99:A:LEU:HD22  | 1:103:A:GLY:H    | 6        | 0.37          |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG12 | 7        | 0.37          |
| (1,1519) | 1:66:A:VAL:HG13  | 1:89:A:VAL:HG11  | 17       | 0.37          |
| (1,1510) | 1:115:A:HIS:HB3  | 1:167:A:THR:HG21 | 1        | 0.37          |
| (1,1456) | 1:157:A:VAL:HG21 | 1:151:A:ILE:HG13 | 4        | 0.37          |
| (1,1456) | 1:157:A:VAL:HG22 | 1:151:A:ILE:HG13 | 4        | 0.37          |
| (1,1456) | 1:157:A:VAL:HG23 | 1:151:A:ILE:HG13 | 4        | 0.37          |
| (1,1436) | 1:156:A:LYS:HG3  | 1:157:A:VAL:H    | 11       | 0.37          |
| (1,1422) | 1:145:A:LEU:HD21 | 1:145:A:LEU:H    | 17       | 0.37          |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 19       | 0.37          |
| (1,1396) | 1:83:A:ILE:HG23  | 1:90:A:TYR:HD2   | 12       | 0.37          |
| (1,1388) | 1:67:A:LYS:HD3   | 1:66:A:VAL:HG13  | 9        | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 6        | 0.37          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 6        | 0.37          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 6        | 0.37          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 20       | 0.37          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 20       | 0.37          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 20       | 0.37          |
| (1,352)  | 1:124:A:GLY:H    | 1:95:A:LYS:HD2   | 14       | 0.37          |
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2  | 17       | 0.37          |
| (1,243)  | 1:162:A:LYS:H    | 1:162:A:LYS:HE3  | 18       | 0.37          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 1        | 0.37          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 5        | 0.37          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG3  | 11       | 0.37          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 17       | 0.37          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 9        | 0.37          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 10       | 0.37          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 17       | 0.37          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 4        | 0.37          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD11  | 15       | 0.37          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD12  | 15       | 0.37          |
| (1,126)  | 1:74:A:LEU:H     | 1:74:A:LEU:HD13  | 15       | 0.37          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG22 | 3        | 0.37          |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD11 | 19       | 0.37          |
| (1,44)   | 1:160:A:GLY:H    | 1:159:A:PRO:HG2  | 18       | 0.37          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 17       | 0.37          |
| (1,5)    | 1:107:A:ASN:H    | 1:90:A:TYR:HE2   | 1        | 0.37          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG21 | 9        | 0.36          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 9        | 0.36          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 16       | 0.36          |
| (1,2797) | 1:150:A:HIS:HE1  | 1:98:A:GLU:HG2   | 18       | 0.36          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB2   | 9        | 0.36          |
| (1,2014) | 1:77:A:ILE:HD12  | 1:126:A:VAL:HB   | 9        | 0.36          |
| (1,1972) | 1:166:A:ASN:HB2  | 1:169:A:VAL:HG21 | 14       | 0.36          |
| (1,1972) | 1:166:A:ASN:HB2  | 1:169:A:VAL:HG22 | 14       | 0.36          |
| (1,1972) | 1:166:A:ASN:HB2  | 1:169:A:VAL:HG23 | 14       | 0.36          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG21 | 4        | 0.36          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG21 | 17       | 0.36          |
| (1,1844) | 1:108:A:ILE:HA   | 1:109:A:ALA:HB2  | 8        | 0.36          |
| (1,1844) | 1:108:A:ILE:HA   | 1:109:A:ALA:HB1  | 12       | 0.36          |
| (1,1844) | 1:108:A:ILE:HA   | 1:109:A:ALA:HB2  | 16       | 0.36          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 13       | 0.36          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 13       | 0.36          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 13       | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG21  | 20       | 0.36          |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG23 | 15       | 0.36          |
| (1,1519) | 1:131:A:VAL:HG23 | 1:89:A:VAL:HG12  | 6        | 0.36          |
| (1,1510) | 1:115:A:HIS:HB3  | 1:116:A:LEU:HD22 | 9        | 0.36          |
| (1,1497) | 1:130:A:ILE:HG22 | 1:131:A:VAL:H    | 1        | 0.36          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD11  | 10       | 0.36          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD12  | 10       | 0.36          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD13  | 10       | 0.36          |
| (1,1422) | 1:145:A:LEU:HD23 | 1:145:A:LEU:H    | 10       | 0.36          |
| (1,1390) | 1:152:A:LYS:HE2  | 1:148:A:GLU:HB3  | 12       | 0.36          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 3        | 0.36          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 13       | 0.36          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD23 | 13       | 0.36          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 9        | 0.36          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 13       | 0.36          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD13 | 5        | 0.36          |
| (1,159)  | 1:153:A:VAL:H    | 1:154:A:THR:HG22 | 6        | 0.36          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 10       | 0.36          |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG12 | 19       | 0.36          |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 16       | 0.36          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD21 | 13       | 0.36          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 20       | 0.36          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 18       | 0.35          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG22 | 9        | 0.35          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB3  | 7        | 0.35          |
| (1,1877) | 1:112:A:VAL:HA   | 1:90:A:TYR:HB2   | 11       | 0.35          |
| (1,1844) | 1:108:A:ILE:HA   | 1:110:A:ALA:HB1  | 14       | 0.35          |
| (1,1844) | 1:108:A:ILE:HA   | 1:109:A:ALA:HB2  | 19       | 0.35          |
| (1,1843) | 1:147:A:ILE:HD11 | 1:102:A:VAL:HB   | 18       | 0.35          |
| (1,1793) | 1:144:A:LYS:HD3  | 1:147:A:ILE:HG21 | 10       | 0.35          |
| (1,1793) | 1:144:A:LYS:HD3  | 1:147:A:ILE:HG22 | 10       | 0.35          |
| (1,1793) | 1:144:A:LYS:HD3  | 1:147:A:ILE:HG23 | 10       | 0.35          |
| (1,1690) | 1:145:A:LEU:HD21 | 1:67:A:LYS:H     | 2        | 0.35          |
| (1,1690) | 1:145:A:LEU:HD22 | 1:67:A:LYS:H     | 2        | 0.35          |
| (1,1690) | 1:145:A:LEU:HD23 | 1:67:A:LYS:H     | 2        | 0.35          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 2        | 0.35          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 2        | 0.35          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 2        | 0.35          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HD11 | 18       | 0.35          |
| (1,1577) | 1:150:A:HIS:HB3  | 1:154:A:THR:HG22 | 7        | 0.35          |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG22 | 5        | 0.35          |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG21 | 10       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1452) | 1:136:A:LYS:HA   | 1:136:A:LYS:HE3  | 11       | 0.35          |
| (1,1426) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE2  | 16       | 0.35          |
| (1,1422) | 1:145:A:LEU:HD21 | 1:145:A:LEU:H    | 9        | 0.35          |
| (1,1422) | 1:145:A:LEU:HD22 | 1:145:A:LEU:H    | 19       | 0.35          |
| (1,1420) | 1:153:A:VAL:HA   | 1:152:A:LYS:HD3  | 6        | 0.35          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 2        | 0.35          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 2        | 0.35          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 2        | 0.35          |
| (1,1402) | 1:112:A:VAL:HA   | 1:90:A:TYR:HE1   | 11       | 0.35          |
| (1,1400) | 1:99:A:LEU:HD13  | 1:98:A:GLU:HB3   | 3        | 0.35          |
| (1,1391) | 1:144:A:LYS:HB2  | 1:144:A:LYS:HE2  | 16       | 0.35          |
| (1,394)  | 1:121:A:GLU:H    | 1:116:A:LEU:HD22 | 17       | 0.35          |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG12 | 2        | 0.35          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG21 | 12       | 0.35          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 19       | 0.35          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD21 | 2        | 0.35          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD22 | 2        | 0.35          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD23 | 2        | 0.35          |
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2  | 13       | 0.35          |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG2  | 10       | 0.35          |
| (1,236)  | 1:156:A:LYS:H    | 1:156:A:LYS:HE2  | 4        | 0.35          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 18       | 0.35          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD13  | 19       | 0.35          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD11 | 12       | 0.35          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD21 | 10       | 0.35          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD22 | 10       | 0.35          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD23 | 10       | 0.35          |
| (1,159)  | 1:153:A:VAL:H    | 1:154:A:THR:HG21 | 14       | 0.35          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG22 | 17       | 0.35          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 18       | 0.35          |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD22 | 17       | 0.35          |
| (1,90)   | 1:124:A:GLY:H    | 1:77:A:ILE:HG13  | 18       | 0.35          |
| (1,31)   | 1:87:A:SER:H     | 1:134:A:PRO:HB3  | 16       | 0.35          |
| (1,26)   | 1:125:A:SER:H    | 1:92:A:VAL:HB    | 20       | 0.35          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG22 | 2        | 0.34          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG22 | 12       | 0.34          |
| (1,2797) | 1:150:A:HIS:HE1  | 1:98:A:GLU:HB3   | 2        | 0.34          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HB   | 11       | 0.34          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG21 | 12       | 0.34          |
| (1,1999) | 1:98:A:GLU:HG3   | 1:100:A:GLN:HE22 | 13       | 0.34          |
| (1,1962) | 1:162:A:LYS:HE3  | 1:159:A:PRO:HA   | 8        | 0.34          |
| (1,1953) | 1:130:A:ILE:HG22 | 1:88:A:GLY:HA2   | 16       | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1947) | 1:70:A:THR:HB    | 1:67:A:LYS:HB2   | 16       | 0.34          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 12       | 0.34          |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 12       | 0.34          |
| (1,1872) | 1:105:A:SER:HB3  | 1:110:A:ALA:HB3  | 6        | 0.34          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE3   | 20       | 0.34          |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 2        | 0.34          |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 2        | 0.34          |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 2        | 0.34          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 11       | 0.34          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 11       | 0.34          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 11       | 0.34          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 17       | 0.34          |
| (1,1665) | 1:140:A:THR:HG22 | 1:141:A:GLN:H    | 18       | 0.34          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 19       | 0.34          |
| (1,1665) | 1:140:A:THR:HG21 | 1:141:A:GLN:H    | 20       | 0.34          |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 17       | 0.34          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 4        | 0.34          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 4        | 0.34          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 4        | 0.34          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 11       | 0.34          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 13       | 0.34          |
| (1,1551) | 1:99:A:LEU:HD23  | 1:103:A:GLY:H    | 9        | 0.34          |
| (1,1551) | 1:99:A:LEU:HD23  | 1:103:A:GLY:H    | 15       | 0.34          |
| (1,1537) | 1:154:A:THR:HB   | 1:156:A:LYS:HB3  | 10       | 0.34          |
| (1,1535) | 1:75:A:LEU:HD22  | 1:76:A:PRO:HD2   | 15       | 0.34          |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG22  | 19       | 0.34          |
| (1,1511) | 1:128:A:VAL:HG12 | 1:90:A:TYR:H     | 15       | 0.34          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD13  | 12       | 0.34          |
| (1,1470) | 1:159:A:PRO:HD3  | 1:162:A:LYS:HG3  | 3        | 0.34          |
| (1,1433) | 1:170:A:LYS:HD2  | 1:167:A:THR:HG22 | 7        | 0.34          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 3        | 0.34          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 3        | 0.34          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 3        | 0.34          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 9        | 0.34          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 9        | 0.34          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 9        | 0.34          |
| (1,1392) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HD1   | 12       | 0.34          |
| (1,1383) | 1:80:A:ALA:HB1   | 1:83:A:ILE:HG13  | 20       | 0.34          |
| (1,1377) | 1:89:A:VAL:HG22  | 1:131:A:VAL:HG12 | 20       | 0.34          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 20       | 0.34          |
| (1,351)  | 1:100:A:GLN:HE22 | 1:98:A:GLU:HG3   | 13       | 0.34          |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD12  | 20       | 0.34          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2  | 1        | 0.34          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 6        | 0.34          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB1   | 10       | 0.34          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 16       | 0.34          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 8        | 0.34          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 12       | 0.34          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 18       | 0.34          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 20       | 0.34          |
| (1,205)  | 1:153:A:VAL:H    | 1:152:A:LYS:HD2  | 13       | 0.34          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 13       | 0.34          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD13 | 18       | 0.34          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 17       | 0.34          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG22 | 18       | 0.34          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 19       | 0.34          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG21 | 20       | 0.34          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 16       | 0.34          |
| (1,151)  | 1:91:A:ALA:H     | 1:89:A:VAL:HG21  | 5        | 0.34          |
| (1,151)  | 1:91:A:ALA:H     | 1:89:A:VAL:HG22  | 5        | 0.34          |
| (1,151)  | 1:91:A:ALA:H     | 1:89:A:VAL:HG23  | 5        | 0.34          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG21 | 10       | 0.34          |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG12 | 10       | 0.34          |
| (1,99)   | 1:160:A:GLY:H    | 1:157:A:VAL:HG23 | 18       | 0.34          |
| (1,84)   | 1:72:A:THR:H     | 1:66:A:VAL:HG12  | 11       | 0.34          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG3  | 11       | 0.34          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 2        | 0.34          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD22 | 19       | 0.34          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 10       | 0.34          |
| (1,2799) | 1:93:A:TYR:HE1   | 1:69:A:LEU:HD11  | 14       | 0.33          |
| (1,2023) | 1:119:A:VAL:HG12 | 1:167:A:THR:HG23 | 13       | 0.33          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 18       | 0.33          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD22 | 19       | 0.33          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG21  | 11       | 0.33          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE2  | 18       | 0.33          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE2  | 20       | 0.33          |
| (1,1878) | 1:147:A:ILE:HG22 | 1:148:A:GLU:HB2  | 8        | 0.33          |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 19       | 0.33          |
| (1,1862) | 1:144:A:LYS:HE2  | 1:145:A:LEU:H    | 16       | 0.33          |
| (1,1844) | 1:108:A:ILE:HA   | 1:109:A:ALA:HB2  | 18       | 0.33          |
| (1,1843) | 1:147:A:ILE:HD11 | 1:102:A:VAL:HB   | 11       | 0.33          |
| (1,1843) | 1:147:A:ILE:HD12 | 1:144:A:LYS:HG3  | 17       | 0.33          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 9        | 0.33          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 9        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 9        | 0.33          |
| (1,1688) | 1:116:A:LEU:HD21 | 1:93:A:TYR:H     | 13       | 0.33          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 7        | 0.33          |
| (1,1616) | 1:66:A:VAL:HG11  | 1:131:A:VAL:HB   | 20       | 0.33          |
| (1,1616) | 1:66:A:VAL:HG12  | 1:131:A:VAL:HB   | 20       | 0.33          |
| (1,1616) | 1:66:A:VAL:HG13  | 1:131:A:VAL:HB   | 20       | 0.33          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD11 | 19       | 0.33          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD12 | 19       | 0.33          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD13 | 19       | 0.33          |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG23 | 20       | 0.33          |
| (1,1550) | 1:72:A:THR:HG23  | 1:69:A:LEU:HD11  | 9        | 0.33          |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG21  | 14       | 0.33          |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG21  | 17       | 0.33          |
| (1,1497) | 1:130:A:ILE:HG22 | 1:131:A:VAL:H    | 15       | 0.33          |
| (1,1441) | 1:145:A:LEU:HB2  | 1:89:A:VAL:HG12  | 8        | 0.33          |
| (1,396)  | 1:100:A:GLN:H    | 1:98:A:GLU:HB2   | 11       | 0.33          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD23 | 8        | 0.33          |
| (1,347)  | 1:70:A:THR:H     | 1:69:A:LEU:HB2   | 10       | 0.33          |
| (1,305)  | 1:146:A:TRP:HE1  | 1:145:A:LEU:HD21 | 1        | 0.33          |
| (1,305)  | 1:146:A:TRP:HE1  | 1:145:A:LEU:HD22 | 1        | 0.33          |
| (1,305)  | 1:146:A:TRP:HE1  | 1:145:A:LEU:HD23 | 1        | 0.33          |
| (1,302)  | 1:146:A:TRP:HE1  | 1:69:A:LEU:HB3   | 16       | 0.33          |
| (1,280)  | 1:67:A:LYS:H     | 1:67:A:LYS:HG3   | 4        | 0.33          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 8        | 0.33          |
| (1,210)  | 1:116:A:LEU:H    | 1:115:A:HIS:HB2  | 14       | 0.33          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD13  | 3        | 0.33          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD12 | 15       | 0.33          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 7        | 0.33          |
| (1,165)  | 1:77:A:ILE:H     | 1:78:A:THR:HG21  | 7        | 0.33          |
| (1,165)  | 1:77:A:ILE:H     | 1:78:A:THR:HG22  | 13       | 0.33          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 4        | 0.33          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 4        | 0.33          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 4        | 0.33          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG21 | 9        | 0.33          |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2  | 9        | 0.33          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD22 | 12       | 0.33          |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 1        | 0.33          |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 6        | 0.33          |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 17       | 0.33          |
| (1,12)   | 1:75:A:LEU:H     | 1:76:A:PRO:HG3   | 5        | 0.33          |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 14       | 0.33          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 5        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 7        | 0.33          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG23 | 18       | 0.32          |
| (1,2026) | 1:109:A:ALA:HB1  | 1:83:A:ILE:HG21  | 13       | 0.32          |
| (1,2026) | 1:109:A:ALA:HB3  | 1:83:A:ILE:HG23  | 16       | 0.32          |
| (1,2014) | 1:77:A:ILE:HD11  | 1:126:A:VAL:HB   | 10       | 0.32          |
| (1,1962) | 1:162:A:LYS:HE3  | 1:159:A:PRO:HA   | 16       | 0.32          |
| (1,1950) | 1:73:A:GLU:HG2   | 1:74:A:LEU:H     | 11       | 0.32          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 7        | 0.32          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 17       | 0.32          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG23 | 7        | 0.32          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE2  | 1        | 0.32          |
| (1,1878) | 1:147:A:ILE:HG22 | 1:148:A:GLU:HB2  | 17       | 0.32          |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 18       | 0.32          |
| (1,1877) | 1:112:A:VAL:HA   | 1:90:A:TYR:HB2   | 14       | 0.32          |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 19       | 0.32          |
| (1,1728) | 1:140:A:THR:HG21 | 1:141:A:GLN:HG3  | 12       | 0.32          |
| (1,1728) | 1:140:A:THR:HG22 | 1:141:A:GLN:HG3  | 12       | 0.32          |
| (1,1728) | 1:140:A:THR:HG23 | 1:141:A:GLN:HG3  | 12       | 0.32          |
| (1,1702) | 1:99:A:LEU:HD23  | 1:93:A:TYR:HA    | 3        | 0.32          |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 19       | 0.32          |
| (1,1665) | 1:140:A:THR:HG22 | 1:141:A:GLN:H    | 3        | 0.32          |
| (1,1665) | 1:140:A:THR:HG22 | 1:141:A:GLN:H    | 16       | 0.32          |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 4        | 0.32          |
| (1,1612) | 1:148:A:GLU:HG2  | 1:152:A:LYS:HE2  | 17       | 0.32          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG21 | 20       | 0.32          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG23  | 19       | 0.32          |
| (1,1565) | 1:167:A:THR:HA   | 1:168:A:PHE:HB2  | 19       | 0.32          |
| (1,1535) | 1:75:A:LEU:HD23  | 1:76:A:PRO:HD2   | 4        | 0.32          |
| (1,1506) | 1:170:A:LYS:HE2  | 1:171:A:VAL:H    | 13       | 0.32          |
| (1,1506) | 1:156:A:LYS:HE3  | 1:157:A:VAL:H    | 15       | 0.32          |
| (1,1456) | 1:157:A:VAL:HG21 | 1:151:A:ILE:HG13 | 2        | 0.32          |
| (1,1456) | 1:157:A:VAL:HG22 | 1:151:A:ILE:HG13 | 2        | 0.32          |
| (1,1456) | 1:157:A:VAL:HG23 | 1:151:A:ILE:HG13 | 2        | 0.32          |
| (1,1432) | 1:95:A:LYS:HD3   | 1:123:A:CYS:H    | 10       | 0.32          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD11  | 2        | 0.32          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD12  | 2        | 0.32          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD13  | 2        | 0.32          |
| (1,1393) | 1:170:A:LYS:HE3  | 1:170:A:LYS:HG2  | 4        | 0.32          |
| (1,1392) | 1:126:A:VAL:HG23 | 1:90:A:TYR:HD1   | 18       | 0.32          |
| (1,1385) | 1:170:A:LYS:HG2  | 1:170:A:LYS:HE3  | 4        | 0.32          |
| (1,356)  | 1:100:A:GLN:H    | 1:102:A:VAL:HG11 | 12       | 0.32          |
| (1,187)  | 1:151:A:ILE:H    | 1:151:A:ILE:HD11 | 19       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG22 | 3        | 0.32          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG22 | 16       | 0.32          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG2   | 11       | 0.32          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG22 | 2        | 0.32          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 3        | 0.32          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 4        | 0.32          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG22 | 6        | 0.32          |
| (1,111)  | 1:148:A:GLU:H    | 1:148:A:GLU:HG3  | 16       | 0.32          |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2  | 16       | 0.32          |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 12       | 0.32          |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 14       | 0.32          |
| (1,31)   | 1:87:A:SER:H     | 1:134:A:PRO:HB3  | 20       | 0.32          |
| (1,12)   | 1:75:A:LEU:H     | 1:76:A:PRO:HG3   | 8        | 0.32          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 6        | 0.32          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 15       | 0.32          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG22 | 5        | 0.31          |
| (1,2799) | 1:93:A:TYR:HE1   | 1:74:A:LEU:HD23  | 17       | 0.31          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HB   | 20       | 0.31          |
| (1,2011) | 1:151:A:ILE:HD13 | 1:157:A:VAL:H    | 11       | 0.31          |
| (1,1999) | 1:98:A:GLU:HG3   | 1:100:A:GLN:HE22 | 18       | 0.31          |
| (1,1994) | 1:162:A:LYS:HE2  | 1:162:A:LYS:H    | 11       | 0.31          |
| (1,1962) | 1:162:A:LYS:HE3  | 1:159:A:PRO:HA   | 2        | 0.31          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD11 | 5        | 0.31          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD12 | 5        | 0.31          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD13 | 5        | 0.31          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE2  | 5        | 0.31          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE2  | 16       | 0.31          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 11       | 0.31          |
| (1,1878) | 1:147:A:ILE:HG22 | 1:148:A:GLU:HB2  | 9        | 0.31          |
| (1,1862) | 1:144:A:LYS:HE2  | 1:145:A:LEU:H    | 14       | 0.31          |
| (1,1840) | 1:86:A:ALA:HB2   | 1:88:A:GLY:H     | 3        | 0.31          |
| (1,1688) | 1:116:A:LEU:HD22 | 1:93:A:TYR:H     | 15       | 0.31          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD11  | 18       | 0.31          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD12  | 18       | 0.31          |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD13  | 18       | 0.31          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 2        | 0.31          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 2        | 0.31          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 2        | 0.31          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG21  | 5        | 0.31          |
| (1,1565) | 1:167:A:THR:HA   | 1:168:A:PHE:HB2  | 13       | 0.31          |
| (1,1565) | 1:167:A:THR:HA   | 1:168:A:PHE:HB2  | 16       | 0.31          |
| (1,1535) | 1:75:A:LEU:HD22  | 1:76:A:PRO:HD2   | 10       | 0.31          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 16       | 0.31          |
| (1,1464) | 1:152:A:LYS:HA   | 1:152:A:LYS:HG3  | 8        | 0.31          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD11  | 11       | 0.31          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD12  | 11       | 0.31          |
| (1,1442) | 1:73:A:GLU:HB2   | 1:74:A:LEU:HD13  | 11       | 0.31          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 1        | 0.31          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 1        | 0.31          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 1        | 0.31          |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 12       | 0.31          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 7        | 0.31          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 16       | 0.31          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 17       | 0.31          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 17       | 0.31          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 17       | 0.31          |
| (1,351)  | 1:100:A:GLN:HE22 | 1:98:A:GLU:HG3   | 18       | 0.31          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 20       | 0.31          |
| (1,243)  | 1:162:A:LYS:H    | 1:162:A:LYS:HE2  | 11       | 0.31          |
| (1,236)  | 1:156:A:LYS:H    | 1:156:A:LYS:HE2  | 13       | 0.31          |
| (1,210)  | 1:116:A:LEU:H    | 1:112:A:VAL:HA   | 15       | 0.31          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD21 | 17       | 0.31          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD22 | 17       | 0.31          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD23 | 17       | 0.31          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 5        | 0.31          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 11       | 0.31          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 11       | 0.31          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 11       | 0.31          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 18       | 0.31          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 18       | 0.31          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 18       | 0.31          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 6        | 0.31          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 12       | 0.31          |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 7        | 0.31          |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 18       | 0.31          |
| (1,7)    | 1:139:A:LEU:H    | 1:138:A:VAL:HG13 | 6        | 0.31          |
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 3        | 0.31          |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 6        | 0.3           |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 10       | 0.3           |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 16       | 0.3           |
| (1,2027) | 1:70:A:THR:HB    | 1:149:A:GLU:HB3  | 19       | 0.3           |
| (1,2025) | 1:144:A:LYS:HE2  | 1:143:A:TRP:HZ3  | 7        | 0.3           |
| (1,2013) | 1:98:A:GLU:HG2   | 1:98:A:GLU:H     | 20       | 0.3           |
| (1,1999) | 1:98:A:GLU:HG3   | 1:100:A:GLN:HE22 | 9        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1947) | 1:70:A:THR:HB    | 1:67:A:LYS:HB2   | 17       | 0.3           |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 17       | 0.3           |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 1        | 0.3           |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD22 | 4        | 0.3           |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG21  | 13       | 0.3           |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG21 | 13       | 0.3           |
| (1,1881) | 1:169:A:VAL:HG23 | 1:168:A:PHE:H    | 3        | 0.3           |
| (1,1881) | 1:169:A:VAL:HG22 | 1:168:A:PHE:H    | 13       | 0.3           |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 3        | 0.3           |
| (1,1863) | 1:95:A:LYS:HE3   | 1:95:A:LYS:H     | 15       | 0.3           |
| (1,1843) | 1:147:A:ILE:HD12 | 1:102:A:VAL:HB   | 3        | 0.3           |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 12       | 0.3           |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 12       | 0.3           |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 12       | 0.3           |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 7        | 0.3           |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 8        | 0.3           |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG23 | 19       | 0.3           |
| (1,1535) | 1:75:A:LEU:HD23  | 1:76:A:PRO:HD2   | 8        | 0.3           |
| (1,1535) | 1:75:A:LEU:HD22  | 1:76:A:PRO:HD2   | 13       | 0.3           |
| (1,1528) | 1:148:A:GLU:HG2  | 1:157:A:VAL:HG21 | 9        | 0.3           |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 19       | 0.3           |
| (1,1470) | 1:159:A:PRO:HD3  | 1:162:A:LYS:HG3  | 17       | 0.3           |
| (1,1448) | 1:156:A:LYS:HD3  | 1:156:A:LYS:H    | 16       | 0.3           |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 14       | 0.3           |
| (1,410)  | 1:95:A:LYS:H     | 1:95:A:LYS:HE3   | 15       | 0.3           |
| (1,351)  | 1:100:A:GLN:HE22 | 1:98:A:GLU:HG3   | 9        | 0.3           |
| (1,347)  | 1:70:A:THR:H     | 1:69:A:LEU:HB2   | 4        | 0.3           |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD12  | 9        | 0.3           |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 11       | 0.3           |
| (1,295)  | 1:108:A:ILE:H    | 1:87:A:SER:HB3   | 13       | 0.3           |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG22  | 5        | 0.3           |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H    | 7        | 0.3           |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD12  | 2        | 0.3           |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 10       | 0.3           |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 6        | 0.3           |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 6        | 0.3           |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 6        | 0.3           |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD21 | 6        | 0.3           |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD22 | 10       | 0.3           |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 8        | 0.3           |
| (1,44)   | 1:160:A:GLY:H    | 1:159:A:PRO:HG2  | 15       | 0.3           |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 10       | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,5)    | 1:107:A:ASN:H    | 1:107:A:ASN:HD22 | 9        | 0.3           |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 9        | 0.29          |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 15       | 0.29          |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 18       | 0.29          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 8        | 0.29          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG21 | 10       | 0.29          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 15       | 0.29          |
| (1,2026) | 1:109:A:ALA:HB2  | 1:83:A:ILE:HG21  | 14       | 0.29          |
| (1,2025) | 1:144:A:LYS:HE3  | 1:143:A:TRP:HZ3  | 5        | 0.29          |
| (1,2025) | 1:144:A:LYS:HE2  | 1:143:A:TRP:HZ3  | 17       | 0.29          |
| (1,1994) | 1:162:A:LYS:HE2  | 1:162:A:LYS:H    | 2        | 0.29          |
| (1,1984) | 1:69:A:LEU:HD11  | 1:151:A:ILE:H    | 2        | 0.29          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD22 | 2        | 0.29          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 3        | 0.29          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 8        | 0.29          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD22 | 12       | 0.29          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG22 | 5        | 0.29          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG22 | 10       | 0.29          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 8        | 0.29          |
| (1,1877) | 1:112:A:VAL:HA   | 1:90:A:TYR:HB2   | 17       | 0.29          |
| (1,1843) | 1:147:A:ILE:HD13 | 1:144:A:LYS:HG3  | 4        | 0.29          |
| (1,1721) | 1:72:A:THR:HG21  | 1:73:A:GLU:HG2   | 4        | 0.29          |
| (1,1721) | 1:72:A:THR:HG22  | 1:73:A:GLU:HG2   | 4        | 0.29          |
| (1,1721) | 1:72:A:THR:HG23  | 1:73:A:GLU:HG2   | 4        | 0.29          |
| (1,1702) | 1:99:A:LEU:HD23  | 1:93:A:TYR:HA    | 18       | 0.29          |
| (1,1666) | 1:156:A:LYS:HG3  | 1:155:A:GLY:H    | 11       | 0.29          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 11       | 0.29          |
| (1,1565) | 1:167:A:THR:HA   | 1:168:A:PHE:HB2  | 1        | 0.29          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 7        | 0.29          |
| (1,1535) | 1:75:A:LEU:HD21  | 1:76:A:PRO:HD2   | 20       | 0.29          |
| (1,1511) | 1:128:A:VAL:HG13 | 1:90:A:TYR:H     | 20       | 0.29          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD12  | 2        | 0.29          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 9        | 0.29          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD13  | 19       | 0.29          |
| (1,1497) | 1:130:A:ILE:HG23 | 1:131:A:VAL:H    | 3        | 0.29          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD11  | 18       | 0.29          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD12  | 18       | 0.29          |
| (1,1423) | 1:82:A:SER:HB2   | 1:75:A:LEU:HD13  | 18       | 0.29          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 18       | 0.29          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 18       | 0.29          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 18       | 0.29          |
| (1,1393) | 1:170:A:LYS:HE2  | 1:170:A:LYS:HG3  | 19       | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1385) | 1:170:A:LYS:HG3 | 1:170:A:LYS:HE2  | 19       | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG11 | 3        | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG12 | 3        | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG13 | 3        | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG11 | 8        | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG12 | 8        | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG13 | 8        | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG11 | 15       | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG12 | 15       | 0.29          |
| (1,371)  | 1:89:A:VAL:H    | 1:128:A:VAL:HG13 | 15       | 0.29          |
| (1,346)  | 1:155:A:GLY:H   | 1:156:A:LYS:HG3  | 11       | 0.29          |
| (1,337)  | 1:93:A:TYR:H    | 1:77:A:ILE:HD12  | 14       | 0.29          |
| (1,302)  | 1:146:A:TRP:HE1 | 1:69:A:LEU:HB3   | 3        | 0.29          |
| (1,260)  | 1:128:A:VAL:H   | 1:91:A:ALA:HB2   | 2        | 0.29          |
| (1,260)  | 1:128:A:VAL:H   | 1:91:A:ALA:HB2   | 8        | 0.29          |
| (1,260)  | 1:128:A:VAL:H   | 1:91:A:ALA:HB2   | 15       | 0.29          |
| (1,243)  | 1:162:A:LYS:H   | 1:162:A:LYS:HE2  | 2        | 0.29          |
| (1,223)  | 1:140:A:THR:H   | 1:141:A:GLN:HG3  | 6        | 0.29          |
| (1,199)  | 1:81:A:ASP:H    | 1:83:A:ILE:HD11  | 8        | 0.29          |
| (1,166)  | 1:141:A:GLN:H   | 1:140:A:THR:HG23 | 11       | 0.29          |
| (1,135)  | 1:116:A:LEU:H   | 1:92:A:VAL:HG21  | 20       | 0.29          |
| (1,135)  | 1:116:A:LEU:H   | 1:92:A:VAL:HG22  | 20       | 0.29          |
| (1,135)  | 1:116:A:LEU:H   | 1:92:A:VAL:HG23  | 20       | 0.29          |
| (1,121)  | 1:103:A:GLY:H   | 1:102:A:VAL:HG21 | 15       | 0.29          |
| (1,121)  | 1:103:A:GLY:H   | 1:102:A:VAL:HG23 | 18       | 0.29          |
| (1,119)  | 1:123:A:CYS:H   | 1:122:A:LEU:HB2  | 1        | 0.29          |
| (1,119)  | 1:123:A:CYS:H   | 1:122:A:LEU:HB2  | 19       | 0.29          |
| (1,99)   | 1:160:A:GLY:H   | 1:122:A:LEU:HD11 | 19       | 0.29          |
| (1,66)   | 1:123:A:CYS:H   | 1:116:A:LEU:HD21 | 15       | 0.29          |
| (1,63)   | 1:170:A:LYS:H   | 1:170:A:LYS:HE3  | 11       | 0.29          |
| (1,45)   | 1:90:A:TYR:H    | 1:89:A:VAL:HB    | 4        | 0.29          |
| (1,37)   | 1:88:A:GLY:H    | 1:108:A:ILE:HB   | 15       | 0.29          |
| (1,31)   | 1:87:A:SER:H    | 1:106:A:ARG:HB3  | 1        | 0.29          |
| (1,12)   | 1:75:A:LEU:H    | 1:76:A:PRO:HG3   | 6        | 0.29          |
| (1,9)    | 1:79:A:GLU:H    | 1:77:A:ILE:HA    | 6        | 0.29          |
| (1,2820) | 1:168:A:PHE:HZ  | 1:168:A:PHE:HB3  | 4        | 0.28          |
| (1,2820) | 1:168:A:PHE:HZ  | 1:168:A:PHE:HB3  | 7        | 0.28          |
| (1,2820) | 1:168:A:PHE:HZ  | 1:168:A:PHE:HB3  | 14       | 0.28          |
| (1,2789) | 1:90:A:TYR:HD2  | 1:89:A:VAL:HB    | 10       | 0.28          |
| (1,2788) | 1:90:A:TYR:HD1  | 1:126:A:VAL:HG21 | 1        | 0.28          |
| (1,2788) | 1:90:A:TYR:HD1  | 1:126:A:VAL:HG21 | 3        | 0.28          |
| (1,2014) | 1:77:A:ILE:HD13 | 1:126:A:VAL:HB   | 12       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1999) | 1:98:A:GLU:HG3   | 1:100:A:GLN:HE22 | 7        | 0.28          |
| (1,1983) | 1:77:A:ILE:HD12  | 1:125:A:SER:H    | 17       | 0.28          |
| (1,1962) | 1:162:A:LYS:HE3  | 1:159:A:PRO:HA   | 14       | 0.28          |
| (1,1962) | 1:162:A:LYS:HE2  | 1:159:A:PRO:HA   | 18       | 0.28          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD21 | 5        | 0.28          |
| (1,1881) | 1:169:A:VAL:HG22 | 1:168:A:PHE:H    | 4        | 0.28          |
| (1,1864) | 1:147:A:ILE:HG21 | 1:144:A:LYS:HE2  | 7        | 0.28          |
| (1,1864) | 1:147:A:ILE:HG22 | 1:144:A:LYS:HE2  | 7        | 0.28          |
| (1,1864) | 1:147:A:ILE:HG23 | 1:144:A:LYS:HE2  | 7        | 0.28          |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 18       | 0.28          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 8        | 0.28          |
| (1,1668) | 1:172:A:THR:HG21 | 1:172:A:THR:H    | 3        | 0.28          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG23 | 9        | 0.28          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG22 | 14       | 0.28          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG23  | 18       | 0.28          |
| (1,1565) | 1:167:A:THR:HA   | 1:168:A:PHE:HB2  | 5        | 0.28          |
| (1,1535) | 1:75:A:LEU:HD21  | 1:76:A:PRO:HD2   | 17       | 0.28          |
| (1,1508) | 1:169:A:VAL:HB   | 1:170:A:LYS:HD3  | 13       | 0.28          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD13  | 3        | 0.28          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 4        | 0.28          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD13  | 16       | 0.28          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD12  | 17       | 0.28          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 17       | 0.28          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 17       | 0.28          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 17       | 0.28          |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 4        | 0.28          |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 11       | 0.28          |
| (1,1396) | 1:83:A:ILE:HG21  | 1:90:A:TYR:HD2   | 19       | 0.28          |
| (1,1392) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HD1   | 1        | 0.28          |
| (1,1392) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HD1   | 3        | 0.28          |
| (1,1383) | 1:80:A:ALA:HB3   | 1:83:A:ILE:HG13  | 3        | 0.28          |
| (1,351)  | 1:100:A:GLN:HE22 | 1:98:A:GLU:HG3   | 7        | 0.28          |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD13  | 1        | 0.28          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 18       | 0.28          |
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2  | 18       | 0.28          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD13  | 10       | 0.28          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 8        | 0.28          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 5        | 0.28          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 15       | 0.28          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG23 | 5        | 0.28          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 13       | 0.28          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 13       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 13       | 0.28          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG22 | 7        | 0.28          |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG22 | 5        | 0.28          |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2  | 10       | 0.28          |
| (1,67)   | 1:157:A:VAL:H    | 1:100:A:GLN:HG3  | 15       | 0.28          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 8        | 0.28          |
| (1,45)   | 1:90:A:TYR:H     | 1:89:A:VAL:HB    | 3        | 0.28          |
| (1,26)   | 1:125:A:SER:H    | 1:95:A:LYS:HD2   | 1        | 0.28          |
| (1,26)   | 1:125:A:SER:H    | 1:92:A:VAL:HB    | 14       | 0.28          |
| (1,12)   | 1:75:A:LEU:H     | 1:76:A:PRO:HG3   | 1        | 0.28          |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 2        | 0.28          |
| (1,7)    | 1:139:A:LEU:H    | 1:138:A:VAL:HG13 | 20       | 0.28          |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 5        | 0.27          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 2        | 0.27          |
| (1,2799) | 1:93:A:TYR:HE1   | 1:69:A:LEU:HD12  | 8        | 0.27          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG23 | 4        | 0.27          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG23 | 13       | 0.27          |
| (1,2025) | 1:144:A:LYS:HE2  | 1:143:A:TRP:HZ3  | 11       | 0.27          |
| (1,1983) | 1:77:A:ILE:HD11  | 1:125:A:SER:H    | 15       | 0.27          |
| (1,1962) | 1:162:A:LYS:HE3  | 1:159:A:PRO:HA   | 3        | 0.27          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 13       | 0.27          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD22 | 11       | 0.27          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD21 | 15       | 0.27          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG21 | 20       | 0.27          |
| (1,1907) | 1:77:A:ILE:HA    | 1:79:A:GLU:HB2   | 14       | 0.27          |
| (1,1881) | 1:169:A:VAL:HG21 | 1:168:A:PHE:H    | 9        | 0.27          |
| (1,1864) | 1:147:A:ILE:HG21 | 1:144:A:LYS:HE2  | 13       | 0.27          |
| (1,1864) | 1:147:A:ILE:HG22 | 1:144:A:LYS:HE2  | 13       | 0.27          |
| (1,1864) | 1:147:A:ILE:HG23 | 1:144:A:LYS:HE2  | 13       | 0.27          |
| (1,1850) | 1:147:A:ILE:HD11 | 1:148:A:GLU:HG3  | 3        | 0.27          |
| (1,1817) | 1:145:A:LEU:HG   | 1:141:A:GLN:HG2  | 11       | 0.27          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG21 | 7        | 0.27          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG22 | 7        | 0.27          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG23 | 7        | 0.27          |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 9        | 0.27          |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 9        | 0.27          |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 9        | 0.27          |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 16       | 0.27          |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 16       | 0.27          |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 16       | 0.27          |
| (1,1702) | 1:99:A:LEU:HD23  | 1:93:A:TYR:HA    | 20       | 0.27          |
| (1,1688) | 1:116:A:LEU:HD21 | 1:93:A:TYR:H     | 3        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1665) | 1:140:A:THR:HG21 | 1:141:A:GLN:H    | 13       | 0.27          |
| (1,1659) | 1:104:A:ILE:HG23 | 1:143:A:TRP:HA   | 4        | 0.27          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG21  | 14       | 0.27          |
| (1,1565) | 1:167:A:THR:HA   | 1:168:A:PHE:HB2  | 11       | 0.27          |
| (1,1544) | 1:173:A:LEU:HD11 | 1:173:A:LEU:HA   | 3        | 0.27          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 1        | 0.27          |
| (1,1487) | 1:126:A:VAL:HA   | 1:92:A:VAL:HB    | 12       | 0.27          |
| (1,1455) | 1:170:A:LYS:HG3  | 1:169:A:VAL:HA   | 8        | 0.27          |
| (1,1396) | 1:83:A:ILE:HG23  | 1:90:A:TYR:HD2   | 18       | 0.27          |
| (1,1392) | 1:126:A:VAL:HG23 | 1:90:A:TYR:HD1   | 4        | 0.27          |
| (1,1392) | 1:126:A:VAL:HG23 | 1:90:A:TYR:HD1   | 13       | 0.27          |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG11 | 17       | 0.27          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 16       | 0.27          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 1        | 0.27          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 10       | 0.27          |
| (1,280)  | 1:67:A:LYS:H     | 1:67:A:LYS:HG3   | 20       | 0.27          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB2   | 9        | 0.27          |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H    | 14       | 0.27          |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H    | 20       | 0.27          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG21 | 13       | 0.27          |
| (1,165)  | 1:77:A:ILE:H     | 1:78:A:THR:HG23  | 19       | 0.27          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 17       | 0.27          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG21 | 10       | 0.27          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG22 | 10       | 0.27          |
| (1,152)  | 1:86:A:ALA:H     | 1:128:A:VAL:HG23 | 10       | 0.27          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 15       | 0.27          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 3        | 0.27          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 3        | 0.27          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 3        | 0.27          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 16       | 0.27          |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD13 | 11       | 0.27          |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG21 | 14       | 0.27          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 16       | 0.27          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD23 | 12       | 0.27          |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 19       | 0.27          |
| (1,2826) | 1:143:A:TRP:HZ2  | 1:147:A:ILE:HD12 | 3        | 0.26          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG22 | 17       | 0.26          |
| (1,2801) | 1:168:A:PHE:HE2  | 1:119:A:VAL:HB   | 1        | 0.26          |
| (1,2791) | 1:90:A:TYR:HE1   | 1:112:A:VAL:HG22 | 3        | 0.26          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 5        | 0.26          |
| (1,2026) | 1:109:A:ALA:HB1  | 1:83:A:ILE:HG21  | 11       | 0.26          |
| (1,1962) | 1:162:A:LYS:HE3  | 1:159:A:PRO:HA   | 11       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1962) | 1:162:A:LYS:HE3  | 1:159:A:PRO:HA   | 17       | 0.26          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD21 | 14       | 0.26          |
| (1,1909) | 1:170:A:LYS:HA   | 1:171:A:VAL:HG13 | 15       | 0.26          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 9        | 0.26          |
| (1,1881) | 1:169:A:VAL:HG21 | 1:168:A:PHE:H    | 8        | 0.26          |
| (1,1862) | 1:144:A:LYS:HE2  | 1:145:A:LEU:H    | 6        | 0.26          |
| (1,1862) | 1:144:A:LYS:HE2  | 1:145:A:LEU:H    | 8        | 0.26          |
| (1,1850) | 1:147:A:ILE:HD13 | 1:148:A:GLU:HG3  | 19       | 0.26          |
| (1,1834) | 1:147:A:ILE:HD12 | 1:143:A:TRP:HZ2  | 3        | 0.26          |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HB3  | 15       | 0.26          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG23 | 6        | 0.26          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:75:A:LEU:HD12  | 9        | 0.26          |
| (1,1535) | 1:75:A:LEU:HD23  | 1:76:A:PRO:HD2   | 7        | 0.26          |
| (1,1456) | 1:157:A:VAL:HG11 | 1:151:A:ILE:HG13 | 13       | 0.26          |
| (1,1456) | 1:157:A:VAL:HG12 | 1:151:A:ILE:HG13 | 13       | 0.26          |
| (1,1456) | 1:157:A:VAL:HG13 | 1:151:A:ILE:HG13 | 13       | 0.26          |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 2        | 0.26          |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 3        | 0.26          |
| (1,1399) | 1:138:A:VAL:HG23 | 1:137:A:ALA:H    | 6        | 0.26          |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 14       | 0.26          |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 18       | 0.26          |
| (1,396)  | 1:100:A:GLN:H    | 1:98:A:GLU:HB2   | 5        | 0.26          |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG13 | 18       | 0.26          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD23 | 3        | 0.26          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD22 | 4        | 0.26          |
| (1,306)  | 1:128:A:VAL:H    | 1:72:A:THR:HA    | 10       | 0.26          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG22  | 8        | 0.26          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB2   | 5        | 0.26          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB3   | 6        | 0.26          |
| (1,210)  | 1:116:A:LEU:H    | 1:112:A:VAL:HA   | 1        | 0.26          |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD12  | 17       | 0.26          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 20       | 0.26          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG23 | 11       | 0.26          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 12       | 0.26          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 12       | 0.26          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 12       | 0.26          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 2        | 0.26          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 3        | 0.26          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 4        | 0.26          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 20       | 0.26          |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG13 | 1        | 0.26          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD23 | 8        | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 10       | 0.26          |
| (1,9)    | 1:79:A:GLU:H     | 1:77:A:ILE:HA    | 12       | 0.26          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG22 | 1        | 0.25          |
| (1,2025) | 1:144:A:LYS:HE3  | 1:143:A:TRP:HZ3  | 9        | 0.25          |
| (1,1948) | 1:87:A:SER:HB3   | 1:131:A:VAL:H    | 7        | 0.25          |
| (1,1948) | 1:87:A:SER:HB3   | 1:131:A:VAL:H    | 18       | 0.25          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 9        | 0.25          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 9        | 0.25          |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 13       | 0.25          |
| (1,1864) | 1:147:A:ILE:HG21 | 1:144:A:LYS:HE3  | 9        | 0.25          |
| (1,1864) | 1:147:A:ILE:HG22 | 1:144:A:LYS:HE3  | 9        | 0.25          |
| (1,1864) | 1:147:A:ILE:HG23 | 1:144:A:LYS:HE3  | 9        | 0.25          |
| (1,1829) | 1:84:A:PRO:HD3   | 1:83:A:ILE:HG22  | 12       | 0.25          |
| (1,1801) | 1:159:A:PRO:HG3  | 1:162:A:LYS:HE2  | 18       | 0.25          |
| (1,1753) | 1:106:A:ARG:HG3  | 1:87:A:SER:HB2   | 15       | 0.25          |
| (1,1702) | 1:99:A:LEU:HD21  | 1:93:A:TYR:HA    | 5        | 0.25          |
| (1,1702) | 1:99:A:LEU:HD21  | 1:93:A:TYR:HA    | 17       | 0.25          |
| (1,1659) | 1:104:A:ILE:HG23 | 1:143:A:TRP:HB3  | 5        | 0.25          |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HB3  | 18       | 0.25          |
| (1,1645) | 1:108:A:ILE:HG22 | 1:84:A:PRO:HD2   | 14       | 0.25          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 6        | 0.25          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 16       | 0.25          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 17       | 0.25          |
| (1,1567) | 1:89:A:VAL:HB    | 1:104:A:ILE:HG21 | 11       | 0.25          |
| (1,1539) | 1:69:A:LEU:HD12  | 1:150:A:HIS:HA   | 5        | 0.25          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 14       | 0.25          |
| (1,1448) | 1:156:A:LYS:HD3  | 1:156:A:LYS:H    | 14       | 0.25          |
| (1,1433) | 1:136:A:LYS:HD2  | 1:104:A:ILE:HG22 | 11       | 0.25          |
| (1,1396) | 1:83:A:ILE:HG22  | 1:90:A:TYR:HD2   | 11       | 0.25          |
| (1,1390) | 1:152:A:LYS:HE2  | 1:148:A:GLU:HB3  | 18       | 0.25          |
| (1,1383) | 1:80:A:ALA:HB3   | 1:83:A:ILE:HG13  | 18       | 0.25          |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG11 | 19       | 0.25          |
| (1,338)  | 1:154:A:THR:H    | 1:151:A:ILE:HG22 | 20       | 0.25          |
| (1,295)  | 1:108:A:ILE:H    | 1:87:A:SER:HB2   | 1        | 0.25          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG22  | 3        | 0.25          |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG2  | 14       | 0.25          |
| (1,223)  | 1:140:A:THR:H    | 1:141:A:GLN:HG2  | 20       | 0.25          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 9        | 0.25          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 7        | 0.25          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 7        | 0.25          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 7        | 0.25          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 13       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 7        | 0.25          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 10       | 0.25          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 14       | 0.25          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 15       | 0.25          |
| (1,90)   | 1:124:A:GLY:H    | 1:77:A:ILE:HG13  | 4        | 0.25          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG23 | 20       | 0.25          |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG12 | 9        | 0.25          |
| (1,84)   | 1:72:A:THR:H     | 1:69:A:LEU:HG    | 8        | 0.25          |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD11 | 17       | 0.25          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HB3   | 3        | 0.25          |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 9        | 0.24          |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 16       | 0.24          |
| (1,2820) | 1:168:A:PHE:HZ   | 1:168:A:PHE:HB3  | 19       | 0.24          |
| (1,2026) | 1:109:A:ALA:HB2  | 1:83:A:ILE:HG23  | 19       | 0.24          |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 18       | 0.24          |
| (1,1983) | 1:77:A:ILE:HD12  | 1:125:A:SER:H    | 19       | 0.24          |
| (1,1953) | 1:83:A:ILE:HG22  | 1:128:A:VAL:HA   | 20       | 0.24          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG21 | 8        | 0.24          |
| (1,1909) | 1:170:A:LYS:HA   | 1:171:A:VAL:HG12 | 19       | 0.24          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 19       | 0.24          |
| (1,1864) | 1:147:A:ILE:HG21 | 1:144:A:LYS:HE2  | 20       | 0.24          |
| (1,1864) | 1:147:A:ILE:HG22 | 1:144:A:LYS:HE2  | 20       | 0.24          |
| (1,1864) | 1:147:A:ILE:HG23 | 1:144:A:LYS:HE2  | 20       | 0.24          |
| (1,1801) | 1:159:A:PRO:HG3  | 1:162:A:LYS:HE2  | 5        | 0.24          |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 20       | 0.24          |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 20       | 0.24          |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 20       | 0.24          |
| (1,1725) | 1:86:A:ALA:HB3   | 1:84:A:PRO:HB3   | 7        | 0.24          |
| (1,1702) | 1:99:A:LEU:HD23  | 1:93:A:TYR:HA    | 12       | 0.24          |
| (1,1679) | 1:74:A:LEU:HD21  | 1:76:A:PRO:HG3   | 15       | 0.24          |
| (1,1618) | 1:121:A:GLU:HG2  | 1:94:A:ASP:HB3   | 6        | 0.24          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 3        | 0.24          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 3        | 0.24          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 3        | 0.24          |
| (1,1586) | 1:95:A:LYS:HD3   | 1:95:A:LYS:H     | 14       | 0.24          |
| (1,1552) | 1:111:A:SER:HA   | 1:114:A:ALA:H    | 16       | 0.24          |
| (1,1551) | 1:99:A:LEU:HD22  | 1:103:A:GLY:H    | 17       | 0.24          |
| (1,1535) | 1:75:A:LEU:HD22  | 1:76:A:PRO:HD2   | 19       | 0.24          |
| (1,1511) | 1:128:A:VAL:HG11 | 1:90:A:TYR:H     | 14       | 0.24          |
| (1,1506) | 1:156:A:LYS:HE2  | 1:157:A:VAL:H    | 10       | 0.24          |
| (1,1504) | 1:147:A:ILE:HD11 | 1:157:A:VAL:HG21 | 14       | 0.24          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 20       | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD21  | 10       | 0.24          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD22  | 10       | 0.24          |
| (1,1409) | 1:73:A:GLU:HG3   | 1:74:A:LEU:HD23  | 10       | 0.24          |
| (1,1402) | 1:112:A:VAL:HA   | 1:90:A:TYR:HE1   | 19       | 0.24          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 9        | 0.24          |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD13  | 4        | 0.24          |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD11  | 16       | 0.24          |
| (1,311)  | 1:88:A:GLY:H     | 1:106:A:ARG:HD3  | 13       | 0.24          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 7        | 0.24          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 5        | 0.24          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB1   | 17       | 0.24          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB3   | 20       | 0.24          |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H    | 18       | 0.24          |
| (1,231)  | 1:140:A:THR:H    | 1:136:A:LYS:HE2  | 6        | 0.24          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 3        | 0.24          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 17       | 0.24          |
| (1,148)  | 1:91:A:ALA:H     | 1:128:A:VAL:HB   | 16       | 0.24          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 6        | 0.24          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 8        | 0.24          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 9        | 0.24          |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD12 | 1        | 0.24          |
| (1,86)   | 1:170:A:LYS:H    | 1:169:A:VAL:HG11 | 19       | 0.24          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD22 | 4        | 0.24          |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD13 | 16       | 0.24          |
| (1,63)   | 1:170:A:LYS:H    | 1:170:A:LYS:HE2  | 13       | 0.24          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 3        | 0.24          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 1        | 0.24          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD21 | 3        | 0.24          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD23 | 5        | 0.24          |
| (1,12)   | 1:75:A:LEU:H     | 1:76:A:PRO:HG3   | 13       | 0.24          |
| (1,12)   | 1:75:A:LEU:H     | 1:76:A:PRO:HG3   | 20       | 0.24          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG22 | 14       | 0.23          |
| (1,2812) | 1:90:A:TYR:HD2   | 1:104:A:ILE:HG23 | 19       | 0.23          |
| (1,1983) | 1:77:A:ILE:HD11  | 1:125:A:SER:H    | 2        | 0.23          |
| (1,1983) | 1:77:A:ILE:HD11  | 1:125:A:SER:H    | 16       | 0.23          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG23 | 12       | 0.23          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE3  | 11       | 0.23          |
| (1,1881) | 1:169:A:VAL:HG21 | 1:168:A:PHE:H    | 11       | 0.23          |
| (1,1840) | 1:86:A:ALA:HB3   | 1:88:A:GLY:H     | 7        | 0.23          |
| (1,1804) | 1:123:A:CYS:HB3  | 1:95:A:LYS:HE3   | 13       | 0.23          |
| (1,1801) | 1:159:A:PRO:HG3  | 1:162:A:LYS:HE3  | 11       | 0.23          |
| (1,1690) | 1:145:A:LEU:HD21 | 1:67:A:LYS:H     | 18       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1690) | 1:145:A:LEU:HD22 | 1:67:A:LYS:H     | 18       | 0.23          |
| (1,1690) | 1:145:A:LEU:HD23 | 1:67:A:LYS:H     | 18       | 0.23          |
| (1,1676) | 1:69:A:LEU:HD23  | 1:149:A:GLU:HB3  | 14       | 0.23          |
| (1,1676) | 1:69:A:LEU:HD21  | 1:149:A:GLU:HB3  | 19       | 0.23          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 19       | 0.23          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 19       | 0.23          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 19       | 0.23          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG21 | 11       | 0.23          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 2        | 0.23          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG23  | 4        | 0.23          |
| (1,1578) | 1:77:A:ILE:HG12  | 1:124:A:GLY:H    | 2        | 0.23          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 3        | 0.23          |
| (1,1528) | 1:148:A:GLU:HG2  | 1:147:A:ILE:HB   | 13       | 0.23          |
| (1,1519) | 1:66:A:VAL:HG12  | 1:89:A:VAL:HG23  | 19       | 0.23          |
| (1,1514) | 1:147:A:ILE:HD12 | 1:157:A:VAL:H    | 19       | 0.23          |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG21  | 13       | 0.23          |
| (1,1450) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HB2   | 5        | 0.23          |
| (1,1399) | 1:138:A:VAL:HG22 | 1:137:A:ALA:H    | 10       | 0.23          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 2        | 0.23          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 19       | 0.23          |
| (1,394)  | 1:121:A:GLU:H    | 1:116:A:LEU:HD22 | 2        | 0.23          |
| (1,345)  | 1:124:A:GLY:H    | 1:77:A:ILE:HG12  | 2        | 0.23          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 8        | 0.23          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD21 | 18       | 0.23          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD22 | 18       | 0.23          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD23 | 18       | 0.23          |
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2  | 2        | 0.23          |
| (1,275)  | 1:150:A:HIS:H    | 1:149:A:GLU:HB2  | 13       | 0.23          |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H    | 5        | 0.23          |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H    | 6        | 0.23          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG21 | 20       | 0.23          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG22 | 20       | 0.23          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG23 | 20       | 0.23          |
| (1,148)  | 1:91:A:ALA:H     | 1:126:A:VAL:HB   | 20       | 0.23          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG22 | 2        | 0.23          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 12       | 0.23          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 13       | 0.23          |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD21 | 19       | 0.23          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG22 | 13       | 0.23          |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2  | 7        | 0.23          |
| (1,44)   | 1:160:A:GLY:H    | 1:159:A:PRO:HG2  | 5        | 0.23          |
| (1,2799) | 1:93:A:TYR:HE1   | 1:74:A:LEU:HD23  | 12       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2799) | 1:93:A:TYR:HE2   | 1:74:A:LEU:HD22  | 19       | 0.22          |
| (1,2795) | 1:93:A:TYR:HD2   | 1:91:A:ALA:HB3   | 6        | 0.22          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 2        | 0.22          |
| (1,1861) | 1:104:A:ILE:HD11 | 1:140:A:THR:H    | 3        | 0.22          |
| (1,1861) | 1:104:A:ILE:HD11 | 1:140:A:THR:H    | 14       | 0.22          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 19       | 0.22          |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 3        | 0.22          |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 3        | 0.22          |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 3        | 0.22          |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB3  | 15       | 0.22          |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB3  | 15       | 0.22          |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB3  | 15       | 0.22          |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 20       | 0.22          |
| (1,1665) | 1:140:A:THR:HG23 | 1:141:A:GLN:H    | 12       | 0.22          |
| (1,1596) | 1:77:A:ILE:HG21  | 1:123:A:CYS:HB2  | 7        | 0.22          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD21 | 10       | 0.22          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD22 | 10       | 0.22          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD23 | 10       | 0.22          |
| (1,1552) | 1:111:A:SER:HA   | 1:114:A:ALA:H    | 3        | 0.22          |
| (1,1551) | 1:99:A:LEU:HD21  | 1:103:A:GLY:H    | 18       | 0.22          |
| (1,1539) | 1:69:A:LEU:HD13  | 1:150:A:HIS:HA   | 9        | 0.22          |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG21 | 13       | 0.22          |
| (1,1511) | 1:128:A:VAL:HG11 | 1:90:A:TYR:H     | 18       | 0.22          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD13  | 5        | 0.22          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 8        | 0.22          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD13  | 10       | 0.22          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 18       | 0.22          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD21  | 8        | 0.22          |
| (1,1470) | 1:159:A:PRO:HD3  | 1:162:A:LYS:HG3  | 14       | 0.22          |
| (1,1448) | 1:156:A:LYS:HD3  | 1:156:A:LYS:H    | 2        | 0.22          |
| (1,1400) | 1:99:A:LEU:HD13  | 1:149:A:GLU:HG3  | 2        | 0.22          |
| (1,1399) | 1:138:A:VAL:HG21 | 1:137:A:ALA:H    | 8        | 0.22          |
| (1,1396) | 1:83:A:ILE:HG23  | 1:90:A:TYR:HD2   | 8        | 0.22          |
| (1,1383) | 1:80:A:ALA:HB2   | 1:83:A:ILE:HG13  | 19       | 0.22          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 15       | 0.22          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD21 | 5        | 0.22          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 14       | 0.22          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG23  | 12       | 0.22          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB1   | 4        | 0.22          |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG2  | 17       | 0.22          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 19       | 0.22          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG23 | 12       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 12       | 0.22          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 18       | 0.22          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 6        | 0.22          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 20       | 0.22          |
| (1,148)  | 1:91:A:ALA:H     | 1:128:A:VAL:HB   | 9        | 0.22          |
| (1,121)  | 1:103:A:GLY:H    | 1:102:A:VAL:HG23 | 17       | 0.22          |
| (1,119)  | 1:123:A:CYS:H    | 1:122:A:LEU:HB2  | 18       | 0.22          |
| (1,88)   | 1:90:A:TYR:H     | 1:104:A:ILE:HG21 | 11       | 0.22          |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 4        | 0.22          |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 5        | 0.21          |
| (1,2026) | 1:109:A:ALA:HB3  | 1:83:A:ILE:HG22  | 3        | 0.21          |
| (1,2013) | 1:98:A:GLU:HG2   | 1:98:A:GLU:H     | 15       | 0.21          |
| (1,1984) | 1:69:A:LEU:HD13  | 1:151:A:ILE:H    | 9        | 0.21          |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 5        | 0.21          |
| (1,1983) | 1:77:A:ILE:HD12  | 1:125:A:SER:H    | 9        | 0.21          |
| (1,1948) | 1:87:A:SER:HB3   | 1:131:A:VAL:H    | 14       | 0.21          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG21 | 18       | 0.21          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE2  | 7        | 0.21          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 3        | 0.21          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 14       | 0.21          |
| (1,1861) | 1:104:A:ILE:HD12 | 1:140:A:THR:H    | 17       | 0.21          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 2        | 0.21          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 7        | 0.21          |
| (1,1702) | 1:99:A:LEU:HD22  | 1:93:A:TYR:HA    | 11       | 0.21          |
| (1,1618) | 1:121:A:GLU:HG3  | 1:94:A:ASP:HB3   | 13       | 0.21          |
| (1,1612) | 1:148:A:GLU:HG2  | 1:152:A:LYS:HE2  | 5        | 0.21          |
| (1,1586) | 1:95:A:LYS:HD3   | 1:95:A:LYS:H     | 20       | 0.21          |
| (1,1578) | 1:77:A:ILE:HG12  | 1:124:A:GLY:H    | 3        | 0.21          |
| (1,1564) | 1:156:A:LYS:HB2  | 1:154:A:THR:HG21 | 7        | 0.21          |
| (1,1551) | 1:99:A:LEU:HD22  | 1:103:A:GLY:H    | 14       | 0.21          |
| (1,1510) | 1:115:A:HIS:HB3  | 1:167:A:THR:HG22 | 16       | 0.21          |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 6        | 0.21          |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 17       | 0.21          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 11       | 0.21          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD11  | 20       | 0.21          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD12  | 20       | 0.21          |
| (1,1423) | 1:82:A:SER:HB3   | 1:75:A:LEU:HD13  | 20       | 0.21          |
| (1,1383) | 1:80:A:ALA:HB2   | 1:83:A:ILE:HG13  | 5        | 0.21          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 11       | 0.21          |
| (1,394)  | 1:121:A:GLU:H    | 1:116:A:LEU:HD22 | 12       | 0.21          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 13       | 0.21          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 13       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 13       | 0.21          |
| (1,347)  | 1:70:A:THR:H     | 1:69:A:LEU:HB2   | 20       | 0.21          |
| (1,345)  | 1:124:A:GLY:H    | 1:77:A:ILE:HG12  | 3        | 0.21          |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD11  | 2        | 0.21          |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD13  | 3        | 0.21          |
| (1,311)  | 1:88:A:GLY:H     | 1:106:A:ARG:HD3  | 9        | 0.21          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 4        | 0.21          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 12       | 0.21          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG23  | 17       | 0.21          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB3   | 12       | 0.21          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 2        | 0.21          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 7        | 0.21          |
| (1,190)  | 1:151:A:ILE:H    | 1:147:A:ILE:HG21 | 16       | 0.21          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD21 | 4        | 0.21          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD22 | 4        | 0.21          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD23 | 4        | 0.21          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 15       | 0.21          |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2  | 20       | 0.21          |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD11 | 12       | 0.21          |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD12 | 15       | 0.21          |
| (1,41)   | 1:126:A:VAL:H    | 1:76:A:PRO:HG3   | 13       | 0.21          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD23 | 6        | 0.21          |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 15       | 0.2           |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 18       | 0.2           |
| (1,2797) | 1:150:A:HIS:HE1  | 1:153:A:VAL:HB   | 4        | 0.2           |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 7        | 0.2           |
| (1,1983) | 1:77:A:ILE:HD11  | 1:125:A:SER:H    | 8        | 0.2           |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 13       | 0.2           |
| (1,1969) | 1:152:A:LYS:HE3  | 1:152:A:LYS:HD2  | 19       | 0.2           |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG21 | 6        | 0.2           |
| (1,1881) | 1:169:A:VAL:HG21 | 1:168:A:PHE:H    | 10       | 0.2           |
| (1,1878) | 1:147:A:ILE:HG21 | 1:148:A:GLU:HB2  | 10       | 0.2           |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 8        | 0.2           |
| (1,1803) | 1:152:A:LYS:HD2  | 1:152:A:LYS:HE3  | 19       | 0.2           |
| (1,1702) | 1:99:A:LEU:HD22  | 1:93:A:TYR:HA    | 9        | 0.2           |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HB3  | 12       | 0.2           |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 14       | 0.2           |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 14       | 0.2           |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 14       | 0.2           |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG23  | 12       | 0.2           |
| (1,1511) | 1:128:A:VAL:HG13 | 1:90:A:TYR:H     | 1        | 0.2           |
| (1,1511) | 1:128:A:VAL:HG13 | 1:90:A:TYR:H     | 5        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD23  | 10       | 0.2           |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG12 | 19       | 0.2           |
| (1,1464) | 1:136:A:LYS:HA   | 1:136:A:LYS:HG2  | 16       | 0.2           |
| (1,1464) | 1:136:A:LYS:HA   | 1:136:A:LYS:HG3  | 17       | 0.2           |
| (1,1402) | 1:112:A:VAL:HA   | 1:115:A:HIS:HD2  | 18       | 0.2           |
| (1,1391) | 1:162:A:LYS:HB3  | 1:162:A:LYS:HE3  | 18       | 0.2           |
| (1,1377) | 1:89:A:VAL:HG23  | 1:139:A:LEU:HD21 | 11       | 0.2           |
| (1,409)  | 1:97:A:ASP:H     | 1:96:A:SER:HB3   | 4        | 0.2           |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD12  | 19       | 0.2           |
| (1,311)  | 1:88:A:GLY:H     | 1:106:A:ARG:HD3  | 7        | 0.2           |
| (1,259)  | 1:146:A:TRP:HE1  | 1:67:A:LYS:HA    | 13       | 0.2           |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H    | 17       | 0.2           |
| (1,199)  | 1:81:A:ASP:H     | 1:83:A:ILE:HD11  | 1        | 0.2           |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 4        | 0.2           |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 8        | 0.2           |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 8        | 0.2           |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 8        | 0.2           |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 8        | 0.2           |
| (1,112)  | 1:87:A:SER:H     | 1:131:A:VAL:HG11 | 15       | 0.2           |
| (1,99)   | 1:160:A:GLY:H    | 1:122:A:LEU:HD12 | 8        | 0.2           |
| (1,95)   | 1:153:A:VAL:H    | 1:152:A:LYS:HB2  | 13       | 0.2           |
| (1,95)   | 1:153:A:VAL:H    | 1:152:A:LYS:HB2  | 20       | 0.2           |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2  | 1        | 0.2           |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD12 | 9        | 0.2           |
| (1,63)   | 1:170:A:LYS:H    | 1:170:A:LYS:HE2  | 20       | 0.2           |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 5        | 0.2           |
| (1,1994) | 1:162:A:LYS:HE2  | 1:162:A:LYS:H    | 17       | 0.19          |
| (1,1969) | 1:152:A:LYS:HE3  | 1:152:A:LYS:HD2  | 12       | 0.19          |
| (1,1964) | 1:133:A:GLU:HG3  | 1:133:A:GLU:H    | 17       | 0.19          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 12       | 0.19          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD11 | 18       | 0.19          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD12 | 18       | 0.19          |
| (1,1914) | 1:68:A:SER:HB2   | 1:145:A:LEU:HD13 | 18       | 0.19          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 8        | 0.19          |
| (1,1862) | 1:144:A:LYS:HE3  | 1:145:A:LEU:H    | 1        | 0.19          |
| (1,1861) | 1:104:A:ILE:HD11 | 1:140:A:THR:H    | 12       | 0.19          |
| (1,1844) | 1:108:A:ILE:HA   | 1:110:A:ALA:HB3  | 13       | 0.19          |
| (1,1803) | 1:152:A:LYS:HD2  | 1:152:A:LYS:HE3  | 12       | 0.19          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 10       | 0.19          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 15       | 0.19          |
| (1,1761) | 1:170:A:LYS:HD2  | 1:170:A:LYS:H    | 5        | 0.19          |
| (1,1752) | 1:116:A:LEU:HG   | 1:112:A:VAL:HA   | 10       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 13       | 0.19          |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 13       | 0.19          |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 13       | 0.19          |
| (1,1729) | 1:102:A:VAL:HG11 | 1:161:A:ASN:HD22 | 12       | 0.19          |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 12       | 0.19          |
| (1,1645) | 1:108:A:ILE:HG23 | 1:84:A:PRO:HD2   | 7        | 0.19          |
| (1,1548) | 1:104:A:ILE:HD11 | 1:144:A:LYS:H    | 15       | 0.19          |
| (1,1535) | 1:75:A:LEU:HD21  | 1:76:A:PRO:HD2   | 3        | 0.19          |
| (1,1511) | 1:128:A:VAL:HG12 | 1:90:A:TYR:H     | 17       | 0.19          |
| (1,1506) | 1:170:A:LYS:HE2  | 1:171:A:VAL:H    | 1        | 0.19          |
| (1,1504) | 1:147:A:ILE:HD12 | 1:157:A:VAL:HG13 | 4        | 0.19          |
| (1,1504) | 1:147:A:ILE:HD11 | 1:157:A:VAL:HG13 | 16       | 0.19          |
| (1,1471) | 1:117:A:LYS:HG2  | 1:112:A:VAL:HG13 | 14       | 0.19          |
| (1,1464) | 1:136:A:LYS:HA   | 1:136:A:LYS:HG2  | 5        | 0.19          |
| (1,1464) | 1:136:A:LYS:HA   | 1:136:A:LYS:HG3  | 9        | 0.19          |
| (1,1456) | 1:157:A:VAL:HG21 | 1:151:A:ILE:HG13 | 16       | 0.19          |
| (1,1456) | 1:157:A:VAL:HG22 | 1:151:A:ILE:HG13 | 16       | 0.19          |
| (1,1456) | 1:157:A:VAL:HG23 | 1:151:A:ILE:HG13 | 16       | 0.19          |
| (1,1435) | 1:84:A:PRO:HG3   | 1:130:A:ILE:HD12 | 7        | 0.19          |
| (1,1396) | 1:83:A:ILE:HG21  | 1:90:A:TYR:HD1   | 10       | 0.19          |
| (1,394)  | 1:121:A:GLU:H    | 1:116:A:LEU:HD23 | 1        | 0.19          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD23 | 9        | 0.19          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 5        | 0.19          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG23  | 15       | 0.19          |
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2  | 5        | 0.19          |
| (1,275)  | 1:150:A:HIS:H    | 1:149:A:GLU:HB3  | 11       | 0.19          |
| (1,244)  | 1:123:A:CYS:H    | 1:95:A:LYS:H     | 4        | 0.19          |
| (1,243)  | 1:162:A:LYS:H    | 1:162:A:LYS:HE2  | 17       | 0.19          |
| (1,235)  | 1:87:A:SER:H     | 1:131:A:VAL:H    | 12       | 0.19          |
| (1,217)  | 1:122:A:LEU:H    | 1:94:A:ASP:HA    | 4        | 0.19          |
| (1,205)  | 1:153:A:VAL:H    | 1:152:A:LYS:HD2  | 19       | 0.19          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 14       | 0.19          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 14       | 0.19          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 14       | 0.19          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG21 | 19       | 0.19          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG22 | 19       | 0.19          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG23 | 19       | 0.19          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 10       | 0.19          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 15       | 0.19          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 1        | 0.19          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 18       | 0.19          |
| (1,150)  | 1:142:A:ALA:H    | 1:145:A:LEU:HB2  | 18       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,149)  | 1:135:A:ASP:H    | 1:133:A:GLU:HG3  | 20       | 0.19          |
| (1,148)  | 1:91:A:ALA:H     | 1:128:A:VAL:HB   | 19       | 0.19          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 12       | 0.19          |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD23 | 7        | 0.19          |
| (1,90)   | 1:124:A:GLY:H    | 1:77:A:ILE:HG13  | 12       | 0.19          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 2        | 0.19          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 13       | 0.19          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 14       | 0.19          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 18       | 0.19          |
| (1,34)   | 1:148:A:GLU:H    | 1:144:A:LYS:HG2  | 15       | 0.19          |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 9        | 0.19          |
| (1,12)   | 1:75:A:LEU:H     | 1:76:A:PRO:HG3   | 15       | 0.19          |
| (1,4)    | 1:142:A:ALA:H    | 1:145:A:LEU:HB2  | 18       | 0.19          |
| (1,2823) | 1:115:A:HIS:HE1  | 1:168:A:PHE:HE1  | 7        | 0.18          |
| (1,2820) | 1:168:A:PHE:HZ   | 1:92:A:VAL:HG11  | 8        | 0.18          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB2   | 5        | 0.18          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG22 | 14       | 0.18          |
| (1,2014) | 1:77:A:ILE:HD13  | 1:126:A:VAL:HB   | 6        | 0.18          |
| (1,1994) | 1:162:A:LYS:HE2  | 1:162:A:LYS:H    | 8        | 0.18          |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 1        | 0.18          |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 3        | 0.18          |
| (1,1965) | 1:83:A:ILE:HD13  | 1:82:A:SER:HA    | 2        | 0.18          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 7        | 0.18          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 9        | 0.18          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 15       | 0.18          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 16       | 0.18          |
| (1,1902) | 1:77:A:ILE:HA    | 1:76:A:PRO:HB3   | 12       | 0.18          |
| (1,1881) | 1:169:A:VAL:HG22 | 1:168:A:PHE:H    | 6        | 0.18          |
| (1,1881) | 1:169:A:VAL:HG22 | 1:168:A:PHE:H    | 18       | 0.18          |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 1        | 0.18          |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 13       | 0.18          |
| (1,1861) | 1:104:A:ILE:HD13 | 1:140:A:THR:H    | 7        | 0.18          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 1        | 0.18          |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 4        | 0.18          |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 4        | 0.18          |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 4        | 0.18          |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB3  | 19       | 0.18          |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB3  | 19       | 0.18          |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB3  | 19       | 0.18          |
| (1,1688) | 1:116:A:LEU:HD21 | 1:93:A:TYR:H     | 8        | 0.18          |
| (1,1645) | 1:108:A:ILE:HG22 | 1:84:A:PRO:HD2   | 20       | 0.18          |
| (1,1616) | 1:66:A:VAL:HG21  | 1:131:A:VAL:HB   | 4        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1616) | 1:66:A:VAL:HG22  | 1:131:A:VAL:HB   | 4        | 0.18          |
| (1,1616) | 1:66:A:VAL:HG23  | 1:131:A:VAL:HB   | 4        | 0.18          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG23  | 15       | 0.18          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 12       | 0.18          |
| (1,1552) | 1:111:A:SER:HA   | 1:114:A:ALA:H    | 5        | 0.18          |
| (1,1551) | 1:99:A:LEU:HD22  | 1:103:A:GLY:H    | 4        | 0.18          |
| (1,1543) | 1:119:A:VAL:HG13 | 1:168:A:PHE:HB3  | 5        | 0.18          |
| (1,1535) | 1:75:A:LEU:HD21  | 1:76:A:PRO:HD2   | 18       | 0.18          |
| (1,1494) | 1:172:A:THR:HB   | 1:173:A:LEU:HD11 | 19       | 0.18          |
| (1,1464) | 1:152:A:LYS:HA   | 1:152:A:LYS:HG3  | 1        | 0.18          |
| (1,1464) | 1:152:A:LYS:HA   | 1:152:A:LYS:HG3  | 19       | 0.18          |
| (1,1448) | 1:156:A:LYS:HD3  | 1:156:A:LYS:H    | 13       | 0.18          |
| (1,1392) | 1:126:A:VAL:HG22 | 1:90:A:TYR:HD1   | 14       | 0.18          |
| (1,1377) | 1:89:A:VAL:HG21  | 1:139:A:LEU:HD22 | 19       | 0.18          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 5        | 0.18          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 17       | 0.18          |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3   | 3        | 0.18          |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3   | 19       | 0.18          |
| (1,353)  | 1:71:A:GLU:H     | 1:69:A:LEU:HB3   | 3        | 0.18          |
| (1,311)  | 1:88:A:GLY:H     | 1:106:A:ARG:HD3  | 2        | 0.18          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 2        | 0.18          |
| (1,302)  | 1:146:A:TRP:HE1  | 1:69:A:LEU:HD12  | 5        | 0.18          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB1   | 18       | 0.18          |
| (1,243)  | 1:162:A:LYS:H    | 1:162:A:LYS:HE2  | 8        | 0.18          |
| (1,229)  | 1:87:A:SER:H     | 1:106:A:ARG:HD3  | 15       | 0.18          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 7        | 0.18          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 7        | 0.18          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 7        | 0.18          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 1        | 0.18          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD21 | 20       | 0.18          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD22 | 20       | 0.18          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD23 | 20       | 0.18          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 7        | 0.18          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 9        | 0.18          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 15       | 0.18          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 16       | 0.18          |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD23 | 15       | 0.18          |
| (1,90)   | 1:124:A:GLY:H    | 1:77:A:ILE:HG13  | 11       | 0.18          |
| (1,84)   | 1:72:A:THR:H     | 1:66:A:VAL:HG11  | 15       | 0.18          |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2  | 2        | 0.18          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 8        | 0.18          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 20       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD22 | 18       | 0.18          |
| (1,9)    | 1:79:A:GLU:H     | 1:77:A:ILE:HA    | 18       | 0.18          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG21 | 11       | 0.17          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG22 | 8        | 0.17          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG21 | 17       | 0.17          |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 12       | 0.17          |
| (1,1953) | 1:83:A:ILE:HG22  | 1:128:A:VAL:HA   | 15       | 0.17          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 6        | 0.17          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 8        | 0.17          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 19       | 0.17          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 20       | 0.17          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 6        | 0.17          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 1        | 0.17          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 14       | 0.17          |
| (1,1882) | 1:125:A:SER:HB3  | 1:97:A:ASP:HA    | 5        | 0.17          |
| (1,1843) | 1:147:A:ILE:HD11 | 1:144:A:LYS:HG3  | 8        | 0.17          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 4        | 0.17          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 9        | 0.17          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 12       | 0.17          |
| (1,1772) | 1:109:A:ALA:HB3  | 1:107:A:ASN:HD22 | 11       | 0.17          |
| (1,1753) | 1:106:A:ARG:HG3  | 1:87:A:SER:HB2   | 14       | 0.17          |
| (1,1724) | 1:122:A:LEU:HD11 | 1:101:A:PHE:H    | 17       | 0.17          |
| (1,1688) | 1:116:A:LEU:HD21 | 1:93:A:TYR:H     | 18       | 0.17          |
| (1,1659) | 1:104:A:ILE:HG23 | 1:143:A:TRP:HB3  | 7        | 0.17          |
| (1,1659) | 1:104:A:ILE:HG22 | 1:143:A:TRP:HB3  | 19       | 0.17          |
| (1,1616) | 1:66:A:VAL:HG21  | 1:131:A:VAL:HB   | 13       | 0.17          |
| (1,1616) | 1:66:A:VAL:HG22  | 1:131:A:VAL:HB   | 13       | 0.17          |
| (1,1616) | 1:66:A:VAL:HG23  | 1:131:A:VAL:HB   | 13       | 0.17          |
| (1,1551) | 1:99:A:LEU:HD22  | 1:103:A:GLY:H    | 16       | 0.17          |
| (1,1548) | 1:104:A:ILE:HD12 | 1:144:A:LYS:H    | 5        | 0.17          |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG23 | 3        | 0.17          |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 4        | 0.17          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD12  | 6        | 0.17          |
| (1,1500) | 1:151:A:ILE:HG23 | 1:152:A:LYS:HE2  | 17       | 0.17          |
| (1,1464) | 1:136:A:LYS:HA   | 1:136:A:LYS:HG3  | 3        | 0.17          |
| (1,1464) | 1:152:A:LYS:HA   | 1:152:A:LYS:HG3  | 20       | 0.17          |
| (1,1450) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HB2   | 18       | 0.17          |
| (1,1392) | 1:126:A:VAL:HG22 | 1:90:A:TYR:HD1   | 8        | 0.17          |
| (1,1392) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HD1   | 17       | 0.17          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 18       | 0.17          |
| (1,513)  | 1:96:A:SER:H     | 1:95:A:LYS:HB2   | 20       | 0.17          |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3   | 7        | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,309)  | 1:88:A:GLY:H    | 1:87:A:SER:HB3   | 16       | 0.17          |
| (1,305)  | 1:146:A:TRP:HE1 | 1:145:A:LEU:HD21 | 2        | 0.17          |
| (1,305)  | 1:146:A:TRP:HE1 | 1:145:A:LEU:HD22 | 2        | 0.17          |
| (1,305)  | 1:146:A:TRP:HE1 | 1:145:A:LEU:HD23 | 2        | 0.17          |
| (1,275)  | 1:150:A:HIS:H   | 1:149:A:GLU:HB2  | 5        | 0.17          |
| (1,237)  | 1:92:A:VAL:H    | 1:90:A:TYR:HB2   | 5        | 0.17          |
| (1,237)  | 1:92:A:VAL:H    | 1:90:A:TYR:HB2   | 15       | 0.17          |
| (1,236)  | 1:156:A:LYS:H   | 1:156:A:LYS:HE3  | 1        | 0.17          |
| (1,203)  | 1:129:A:GLY:H   | 1:128:A:VAL:HG11 | 2        | 0.17          |
| (1,203)  | 1:129:A:GLY:H   | 1:128:A:VAL:HG12 | 2        | 0.17          |
| (1,203)  | 1:129:A:GLY:H   | 1:128:A:VAL:HG13 | 2        | 0.17          |
| (1,203)  | 1:129:A:GLY:H   | 1:128:A:VAL:HG11 | 11       | 0.17          |
| (1,203)  | 1:129:A:GLY:H   | 1:128:A:VAL:HG12 | 11       | 0.17          |
| (1,203)  | 1:129:A:GLY:H   | 1:128:A:VAL:HG13 | 11       | 0.17          |
| (1,197)  | 1:162:A:LYS:H   | 1:162:A:LYS:HD3  | 4        | 0.17          |
| (1,197)  | 1:162:A:LYS:H   | 1:162:A:LYS:HD3  | 9        | 0.17          |
| (1,197)  | 1:162:A:LYS:H   | 1:162:A:LYS:HD3  | 12       | 0.17          |
| (1,165)  | 1:77:A:ILE:H    | 1:77:A:ILE:HG13  | 2        | 0.17          |
| (1,165)  | 1:77:A:ILE:H    | 1:77:A:ILE:HG13  | 14       | 0.17          |
| (1,163)  | 1:112:A:VAL:H   | 1:108:A:ILE:HB   | 11       | 0.17          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG21 | 8        | 0.17          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG22 | 8        | 0.17          |
| (1,152)  | 1:86:A:ALA:H    | 1:128:A:VAL:HG23 | 8        | 0.17          |
| (1,149)  | 1:135:A:ASP:H   | 1:133:A:GLU:HG3  | 6        | 0.17          |
| (1,147)  | 1:74:A:LEU:H    | 1:73:A:GLU:HG3   | 6        | 0.17          |
| (1,147)  | 1:74:A:LEU:H    | 1:73:A:GLU:HG3   | 8        | 0.17          |
| (1,147)  | 1:74:A:LEU:H    | 1:73:A:GLU:HG3   | 19       | 0.17          |
| (1,147)  | 1:74:A:LEU:H    | 1:73:A:GLU:HG3   | 20       | 0.17          |
| (1,119)  | 1:123:A:CYS:H   | 1:122:A:LEU:HB2  | 11       | 0.17          |
| (1,110)  | 1:116:A:LEU:H   | 1:116:A:LEU:HD23 | 14       | 0.17          |
| (1,85)   | 1:125:A:SER:H   | 1:76:A:PRO:HB3   | 10       | 0.17          |
| (1,37)   | 1:88:A:GLY:H    | 1:108:A:ILE:HB   | 7        | 0.17          |
| (1,2823) | 1:115:A:HIS:HE1 | 1:168:A:PHE:HE1  | 14       | 0.16          |
| (1,2799) | 1:93:A:TYR:HE1  | 1:69:A:LEU:HD13  | 1        | 0.16          |
| (1,2795) | 1:93:A:TYR:HD1  | 1:91:A:ALA:HB1   | 7        | 0.16          |
| (1,2788) | 1:90:A:TYR:HD1  | 1:126:A:VAL:HG22 | 7        | 0.16          |
| (1,2656) | 1:86:A:ALA:HB1  | 1:107:A:ASN:HD21 | 20       | 0.16          |
| (1,2656) | 1:86:A:ALA:HB2  | 1:107:A:ASN:HD21 | 20       | 0.16          |
| (1,2656) | 1:86:A:ALA:HB3  | 1:107:A:ASN:HD21 | 20       | 0.16          |
| (1,1984) | 1:69:A:LEU:HD11 | 1:151:A:ILE:H    | 19       | 0.16          |
| (1,1983) | 1:77:A:ILE:HD13 | 1:125:A:SER:H    | 4        | 0.16          |
| (1,1956) | 1:69:A:LEU:HD11 | 1:150:A:HIS:HB3  | 13       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 4        | 0.16          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 13       | 0.16          |
| (1,1948) | 1:87:A:SER:HB3   | 1:131:A:VAL:H    | 20       | 0.16          |
| (1,1911) | 1:85:A:SER:HB3   | 1:83:A:ILE:HG23  | 12       | 0.16          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG23 | 2        | 0.16          |
| (1,1909) | 1:101:A:PHE:HA   | 1:102:A:VAL:HG23 | 3        | 0.16          |
| (1,1904) | 1:100:A:GLN:HA   | 1:156:A:LYS:HG3  | 8        | 0.16          |
| (1,1881) | 1:169:A:VAL:HG23 | 1:168:A:PHE:H    | 16       | 0.16          |
| (1,1877) | 1:112:A:VAL:HA   | 1:115:A:HIS:HB3  | 15       | 0.16          |
| (1,1862) | 1:144:A:LYS:HE2  | 1:145:A:LEU:H    | 17       | 0.16          |
| (1,1844) | 1:108:A:ILE:HA   | 1:110:A:ALA:HB2  | 3        | 0.16          |
| (1,1844) | 1:108:A:ILE:HA   | 1:110:A:ALA:HB3  | 4        | 0.16          |
| (1,1774) | 1:117:A:LYS:HD3  | 1:117:A:LYS:H    | 1        | 0.16          |
| (1,1710) | 1:156:A:LYS:HG3  | 1:100:A:GLN:HA   | 8        | 0.16          |
| (1,1702) | 1:99:A:LEU:HD22  | 1:93:A:TYR:HA    | 19       | 0.16          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG21 | 18       | 0.16          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG22 | 18       | 0.16          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG23 | 18       | 0.16          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG21 | 18       | 0.16          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG22 | 18       | 0.16          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG23 | 18       | 0.16          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG21 | 18       | 0.16          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG22 | 18       | 0.16          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG23 | 18       | 0.16          |
| (1,1688) | 1:116:A:LEU:HD22 | 1:93:A:TYR:H     | 5        | 0.16          |
| (1,1688) | 1:116:A:LEU:HD23 | 1:93:A:TYR:H     | 6        | 0.16          |
| (1,1665) | 1:140:A:THR:HG21 | 1:141:A:GLN:H    | 8        | 0.16          |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HB3  | 8        | 0.16          |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HA   | 13       | 0.16          |
| (1,1659) | 1:104:A:ILE:HG23 | 1:143:A:TRP:HB3  | 17       | 0.16          |
| (1,1640) | 1:159:A:PRO:HB3  | 1:162:A:LYS:HE3  | 14       | 0.16          |
| (1,1618) | 1:121:A:GLU:HG3  | 1:94:A:ASP:HB3   | 15       | 0.16          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 15       | 0.16          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 15       | 0.16          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 15       | 0.16          |
| (1,1584) | 1:95:A:LYS:HD3   | 1:124:A:GLY:H    | 20       | 0.16          |
| (1,1539) | 1:69:A:LEU:HD13  | 1:150:A:HIS:HA   | 17       | 0.16          |
| (1,1537) | 1:154:A:THR:HB   | 1:156:A:LYS:HB3  | 5        | 0.16          |
| (1,1514) | 1:147:A:ILE:HD12 | 1:157:A:VAL:H    | 5        | 0.16          |
| (1,1506) | 1:170:A:LYS:HE2  | 1:171:A:VAL:H    | 19       | 0.16          |
| (1,1487) | 1:126:A:VAL:HA   | 1:92:A:VAL:HB    | 13       | 0.16          |
| (1,1476) | 1:66:A:VAL:HG11  | 1:71:A:GLU:HG3   | 11       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1476) | 1:66:A:VAL:HG12  | 1:71:A:GLU:HG3   | 11       | 0.16          |
| (1,1476) | 1:66:A:VAL:HG13  | 1:71:A:GLU:HG3   | 11       | 0.16          |
| (1,1464) | 1:136:A:LYS:HA   | 1:136:A:LYS:HG2  | 4        | 0.16          |
| (1,1464) | 1:152:A:LYS:HA   | 1:152:A:LYS:HG3  | 14       | 0.16          |
| (1,1448) | 1:156:A:LYS:HD3  | 1:156:A:LYS:H    | 9        | 0.16          |
| (1,1392) | 1:126:A:VAL:HG22 | 1:90:A:TYR:HD1   | 7        | 0.16          |
| (1,1376) | 1:162:A:LYS:HD2  | 1:157:A:VAL:HG23 | 18       | 0.16          |
| (1,352)  | 1:124:A:GLY:H    | 1:95:A:LYS:HD3   | 20       | 0.16          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG22  | 7        | 0.16          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG23  | 19       | 0.16          |
| (1,283)  | 1:117:A:LYS:H    | 1:117:A:LYS:HD3  | 1        | 0.16          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB2   | 14       | 0.16          |
| (1,210)  | 1:116:A:LEU:H    | 1:112:A:VAL:HA   | 13       | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 1        | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 1        | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 1        | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 8        | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 8        | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 8        | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 17       | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 17       | 0.16          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 17       | 0.16          |
| (1,166)  | 1:141:A:GLN:H    | 1:140:A:THR:HG21 | 8        | 0.16          |
| (1,165)  | 1:77:A:ILE:H     | 1:78:A:THR:HG23  | 9        | 0.16          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 4        | 0.16          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 13       | 0.16          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG21 | 13       | 0.16          |
| (1,138)  | 1:150:A:HIS:H    | 1:147:A:ILE:HG22 | 19       | 0.16          |
| (1,73)   | 1:125:A:SER:H    | 1:95:A:LYS:HG3   | 14       | 0.16          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 20       | 0.16          |
| (1,25)   | 1:135:A:ASP:H    | 1:134:A:PRO:HG2  | 13       | 0.16          |
| (1,22)   | 1:88:A:GLY:H     | 1:139:A:LEU:HD23 | 7        | 0.16          |
| (1,7)    | 1:139:A:LEU:H    | 1:138:A:VAL:HG13 | 14       | 0.16          |
| (1,7)    | 1:139:A:LEU:H    | 1:138:A:VAL:HG13 | 18       | 0.16          |
| (1,2868) | 1:115:A:HIS:HE1  | 1:116:A:LEU:HA   | 19       | 0.15          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB2   | 2        | 0.15          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB2   | 13       | 0.15          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 15       | 0.15          |
| (1,2026) | 1:109:A:ALA:HB1  | 1:83:A:ILE:HG22  | 7        | 0.15          |
| (1,2026) | 1:109:A:ALA:HB2  | 1:83:A:ILE:HG22  | 8        | 0.15          |
| (1,1984) | 1:69:A:LEU:HD13  | 1:151:A:ILE:H    | 17       | 0.15          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 10       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 14       | 0.15          |
| (1,1862) | 1:144:A:LYS:HE3  | 1:145:A:LEU:H    | 15       | 0.15          |
| (1,1861) | 1:104:A:ILE:HD12 | 1:140:A:THR:H    | 4        | 0.15          |
| (1,1810) | 1:123:A:CYS:HB2  | 1:95:A:LYS:HD2   | 14       | 0.15          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 20       | 0.15          |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB3  | 5        | 0.15          |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB3  | 5        | 0.15          |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB3  | 5        | 0.15          |
| (1,1659) | 1:104:A:ILE:HG22 | 1:143:A:TRP:HB3  | 11       | 0.15          |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 13       | 0.15          |
| (1,1597) | 1:137:A:ALA:HB1  | 1:141:A:GLN:HG3  | 8        | 0.15          |
| (1,1597) | 1:137:A:ALA:HB2  | 1:141:A:GLN:HG3  | 8        | 0.15          |
| (1,1597) | 1:137:A:ALA:HB3  | 1:141:A:GLN:HG3  | 8        | 0.15          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG22 | 4        | 0.15          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 4        | 0.15          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 10       | 0.15          |
| (1,1548) | 1:104:A:ILE:HD11 | 1:144:A:LYS:H    | 2        | 0.15          |
| (1,1548) | 1:104:A:ILE:HD13 | 1:144:A:LYS:H    | 18       | 0.15          |
| (1,1535) | 1:75:A:LEU:HD22  | 1:76:A:PRO:HD2   | 1        | 0.15          |
| (1,1511) | 1:128:A:VAL:HG13 | 1:90:A:TYR:H     | 7        | 0.15          |
| (1,1508) | 1:169:A:VAL:HB   | 1:168:A:PHE:HB2  | 2        | 0.15          |
| (1,1448) | 1:156:A:LYS:HD2  | 1:156:A:LYS:H    | 6        | 0.15          |
| (1,1402) | 1:112:A:VAL:HA   | 1:90:A:TYR:HE1   | 14       | 0.15          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG11 | 12       | 0.15          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG12 | 12       | 0.15          |
| (1,371)  | 1:89:A:VAL:H     | 1:128:A:VAL:HG13 | 12       | 0.15          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG21  | 13       | 0.15          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG23  | 16       | 0.15          |
| (1,270)  | 1:111:A:SER:H    | 1:115:A:HIS:HD2  | 16       | 0.15          |
| (1,263)  | 1:146:A:TRP:HE1  | 1:68:A:SER:HB3   | 12       | 0.15          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB3   | 1        | 0.15          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB1   | 7        | 0.15          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 13       | 0.15          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 13       | 0.15          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 13       | 0.15          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 13       | 0.15          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 20       | 0.15          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD21 | 9        | 0.15          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD22 | 9        | 0.15          |
| (1,184)  | 1:149:A:GLU:H    | 1:145:A:LEU:HD23 | 9        | 0.15          |
| (1,165)  | 1:77:A:ILE:H     | 1:78:A:THR:HG23  | 6        | 0.15          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 10       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 14       | 0.15          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 1        | 0.15          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 1        | 0.15          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 1        | 0.15          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG21  | 17       | 0.15          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG22  | 17       | 0.15          |
| (1,135)  | 1:116:A:LEU:H    | 1:92:A:VAL:HG23  | 17       | 0.15          |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD22 | 3        | 0.15          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 13       | 0.15          |
| (1,80)   | 1:144:A:LYS:H    | 1:143:A:TRP:HB2  | 15       | 0.15          |
| (1,72)   | 1:153:A:VAL:H    | 1:150:A:HIS:HB2  | 8        | 0.15          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 19       | 0.15          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 17       | 0.15          |
| (1,9)    | 1:79:A:GLU:H     | 1:77:A:ILE:HA    | 17       | 0.15          |
| (1,2873) | 1:150:A:HIS:HE1  | 1:154:A:THR:HG22 | 16       | 0.14          |
| (1,2826) | 1:143:A:TRP:HZ2  | 1:147:A:ILE:HD11 | 5        | 0.14          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB2   | 8        | 0.14          |
| (1,2789) | 1:90:A:TYR:HD2   | 1:89:A:VAL:HB    | 9        | 0.14          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG23 | 5        | 0.14          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG21 | 20       | 0.14          |
| (1,1971) | 1:144:A:LYS:HE2  | 1:144:A:LYS:HG3  | 10       | 0.14          |
| (1,1962) | 1:162:A:LYS:HE2  | 1:159:A:PRO:HA   | 13       | 0.14          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 18       | 0.14          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 5        | 0.14          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB3  | 15       | 0.14          |
| (1,1834) | 1:147:A:ILE:HD11 | 1:143:A:TRP:HZ2  | 5        | 0.14          |
| (1,1829) | 1:84:A:PRO:HD3   | 1:83:A:ILE:HG22  | 16       | 0.14          |
| (1,1826) | 1:167:A:THR:HA   | 1:170:A:LYS:HB3  | 8        | 0.14          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 6        | 0.14          |
| (1,1751) | 1:108:A:ILE:HG23 | 1:111:A:SER:H    | 5        | 0.14          |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB2  | 7        | 0.14          |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB2  | 7        | 0.14          |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB2  | 7        | 0.14          |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB3  | 14       | 0.14          |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB3  | 14       | 0.14          |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB3  | 14       | 0.14          |
| (1,1702) | 1:99:A:LEU:HD21  | 1:93:A:TYR:HA    | 4        | 0.14          |
| (1,1690) | 1:145:A:LEU:HD21 | 1:67:A:LYS:H     | 8        | 0.14          |
| (1,1690) | 1:145:A:LEU:HD22 | 1:67:A:LYS:H     | 8        | 0.14          |
| (1,1690) | 1:145:A:LEU:HD23 | 1:67:A:LYS:H     | 8        | 0.14          |
| (1,1659) | 1:104:A:ILE:HG23 | 1:143:A:TRP:HB3  | 14       | 0.14          |
| (1,1618) | 1:121:A:GLU:HG3  | 1:94:A:ASP:HB3   | 11       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD21 | 5        | 0.14          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD22 | 5        | 0.14          |
| (1,1583) | 1:141:A:GLN:HG3  | 1:145:A:LEU:HD23 | 5        | 0.14          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 3        | 0.14          |
| (1,1566) | 1:119:A:VAL:HG22 | 1:167:A:THR:HG23 | 16       | 0.14          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 19       | 0.14          |
| (1,1555) | 1:148:A:GLU:HG3  | 1:147:A:ILE:HG21 | 14       | 0.14          |
| (1,1551) | 1:99:A:LEU:HD21  | 1:103:A:GLY:H    | 8        | 0.14          |
| (1,1550) | 1:72:A:THR:HG23  | 1:69:A:LEU:HD11  | 4        | 0.14          |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG21 | 4        | 0.14          |
| (1,1513) | 1:102:A:VAL:HG11 | 1:93:A:TYR:HE1   | 9        | 0.14          |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG23  | 3        | 0.14          |
| (1,1511) | 1:128:A:VAL:HG12 | 1:90:A:TYR:H     | 9        | 0.14          |
| (1,1498) | 1:157:A:VAL:HA   | 1:147:A:ILE:HG12 | 18       | 0.14          |
| (1,1487) | 1:126:A:VAL:HA   | 1:75:A:LEU:HB2   | 17       | 0.14          |
| (1,1448) | 1:156:A:LYS:HD3  | 1:156:A:LYS:H    | 8        | 0.14          |
| (1,1425) | 1:139:A:LEU:HD11 | 1:136:A:LYS:HD2  | 12       | 0.14          |
| (1,1425) | 1:139:A:LEU:HD12 | 1:136:A:LYS:HD2  | 12       | 0.14          |
| (1,1425) | 1:139:A:LEU:HD13 | 1:136:A:LYS:HD2  | 12       | 0.14          |
| (1,1392) | 1:126:A:VAL:HG23 | 1:90:A:TYR:HD1   | 5        | 0.14          |
| (1,1392) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HD1   | 20       | 0.14          |
| (1,1376) | 1:162:A:LYS:HD2  | 1:157:A:VAL:HG11 | 16       | 0.14          |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG12 | 9        | 0.14          |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3   | 11       | 0.14          |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3   | 12       | 0.14          |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3   | 15       | 0.14          |
| (1,337)  | 1:93:A:TYR:H     | 1:77:A:ILE:HD12  | 17       | 0.14          |
| (1,332)  | 1:154:A:THR:H    | 1:154:A:THR:HG23 | 18       | 0.14          |
| (1,311)  | 1:88:A:GLY:H     | 1:106:A:ARG:HD3  | 1        | 0.14          |
| (1,309)  | 1:88:A:GLY:H     | 1:87:A:SER:HB3   | 17       | 0.14          |
| (1,285)  | 1:108:A:ILE:H    | 1:83:A:ILE:HG21  | 11       | 0.14          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD21 | 8        | 0.14          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD22 | 8        | 0.14          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD23 | 8        | 0.14          |
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2  | 19       | 0.14          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 1        | 0.14          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 20       | 0.14          |
| (1,244)  | 1:123:A:CYS:H    | 1:95:A:LYS:H     | 8        | 0.14          |
| (1,242)  | 1:94:A:ASP:H     | 1:98:A:GLU:HB2   | 11       | 0.14          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 9        | 0.14          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 9        | 0.14          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 9        | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG21 | 18       | 0.14          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG22 | 18       | 0.14          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG23 | 18       | 0.14          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 6        | 0.14          |
| (1,165)  | 1:77:A:ILE:H     | 1:77:A:ILE:HG13  | 10       | 0.14          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 2        | 0.14          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 3        | 0.14          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 14       | 0.14          |
| (1,149)  | 1:135:A:ASP:H    | 1:133:A:GLU:HG2  | 16       | 0.14          |
| (1,148)  | 1:91:A:ALA:H     | 1:126:A:VAL:HB   | 18       | 0.14          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 18       | 0.14          |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD22 | 16       | 0.14          |
| (1,107)  | 1:118:A:SER:H    | 1:118:A:SER:HB3  | 11       | 0.14          |
| (1,66)   | 1:123:A:CYS:H    | 1:116:A:LEU:HD23 | 9        | 0.14          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 11       | 0.14          |
| (1,61)   | 1:104:A:ILE:H    | 1:101:A:PHE:HE2  | 12       | 0.14          |
| (1,12)   | 1:75:A:LEU:H     | 1:73:A:GLU:HB2   | 3        | 0.14          |
| (1,2869) | 1:115:A:HIS:HE1  | 1:112:A:VAL:HG11 | 19       | 0.13          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB2   | 15       | 0.13          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB1   | 17       | 0.13          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG21 | 2        | 0.13          |
| (1,2656) | 1:86:A:ALA:HB1   | 1:107:A:ASN:HD21 | 5        | 0.13          |
| (1,2656) | 1:86:A:ALA:HB2   | 1:107:A:ASN:HD21 | 5        | 0.13          |
| (1,2656) | 1:86:A:ALA:HB3   | 1:107:A:ASN:HD21 | 5        | 0.13          |
| (1,2026) | 1:109:A:ALA:HB2  | 1:83:A:ILE:HG23  | 12       | 0.13          |
| (1,2013) | 1:98:A:GLU:HG2   | 1:98:A:GLU:H     | 1        | 0.13          |
| (1,1983) | 1:77:A:ILE:HD12  | 1:125:A:SER:H    | 20       | 0.13          |
| (1,1962) | 1:162:A:LYS:HE2  | 1:159:A:PRO:HA   | 19       | 0.13          |
| (1,1950) | 1:73:A:GLU:HG3   | 1:74:A:LEU:H     | 5        | 0.13          |
| (1,1902) | 1:77:A:ILE:HA    | 1:76:A:PRO:HB3   | 10       | 0.13          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB2  | 10       | 0.13          |
| (1,1897) | 1:85:A:SER:HB2   | 1:84:A:PRO:HA    | 6        | 0.13          |
| (1,1887) | 1:77:A:ILE:HA    | 1:117:A:LYS:HE3  | 8        | 0.13          |
| (1,1881) | 1:169:A:VAL:HG22 | 1:168:A:PHE:H    | 5        | 0.13          |
| (1,1881) | 1:169:A:VAL:HG21 | 1:168:A:PHE:H    | 14       | 0.13          |
| (1,1864) | 1:147:A:ILE:HG21 | 1:144:A:LYS:HE3  | 5        | 0.13          |
| (1,1864) | 1:147:A:ILE:HG22 | 1:144:A:LYS:HE3  | 5        | 0.13          |
| (1,1864) | 1:147:A:ILE:HG23 | 1:144:A:LYS:HE3  | 5        | 0.13          |
| (1,1843) | 1:147:A:ILE:HD12 | 1:144:A:LYS:HG3  | 16       | 0.13          |
| (1,1843) | 1:147:A:ILE:HD11 | 1:102:A:VAL:HB   | 19       | 0.13          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 11       | 0.13          |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB3  | 8        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB3  | 8        | 0.13          |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB3  | 8        | 0.13          |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB3  | 12       | 0.13          |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB3  | 12       | 0.13          |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB3  | 12       | 0.13          |
| (1,1702) | 1:99:A:LEU:HD22  | 1:93:A:TYR:HA    | 15       | 0.13          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG21 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG22 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG23 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG21 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG22 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG23 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG21 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG22 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG23 | 6        | 0.13          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG21 | 10       | 0.13          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG22 | 10       | 0.13          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG23 | 10       | 0.13          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG21 | 10       | 0.13          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG22 | 10       | 0.13          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG23 | 10       | 0.13          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG21 | 10       | 0.13          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG22 | 10       | 0.13          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG23 | 10       | 0.13          |
| (1,1690) | 1:145:A:LEU:HD11 | 1:67:A:LYS:H     | 10       | 0.13          |
| (1,1690) | 1:145:A:LEU:HD12 | 1:67:A:LYS:H     | 10       | 0.13          |
| (1,1690) | 1:145:A:LEU:HD13 | 1:67:A:LYS:H     | 10       | 0.13          |
| (1,1688) | 1:116:A:LEU:HD21 | 1:93:A:TYR:H     | 1        | 0.13          |
| (1,1676) | 1:69:A:LEU:HD21  | 1:149:A:GLU:HB3  | 15       | 0.13          |
| (1,1659) | 1:104:A:ILE:HG22 | 1:143:A:TRP:HB3  | 10       | 0.13          |
| (1,1645) | 1:108:A:ILE:HG21 | 1:84:A:PRO:HD2   | 12       | 0.13          |
| (1,1610) | 1:119:A:VAL:HG11 | 1:121:A:GLU:HG2  | 17       | 0.13          |
| (1,1610) | 1:119:A:VAL:HG12 | 1:121:A:GLU:HG2  | 17       | 0.13          |
| (1,1610) | 1:119:A:VAL:HG13 | 1:121:A:GLU:HG2  | 17       | 0.13          |
| (1,1586) | 1:95:A:LYS:HD2   | 1:95:A:LYS:H     | 15       | 0.13          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HD11 | 19       | 0.13          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 9        | 0.13          |
| (1,1552) | 1:111:A:SER:HA   | 1:114:A:ALA:H    | 18       | 0.13          |
| (1,1551) | 1:99:A:LEU:HD21  | 1:103:A:GLY:H    | 20       | 0.13          |
| (1,1535) | 1:75:A:LEU:HD21  | 1:76:A:PRO:HD2   | 6        | 0.13          |
| (1,1511) | 1:128:A:VAL:HG13 | 1:90:A:TYR:H     | 2        | 0.13          |
| (1,1487) | 1:126:A:VAL:HA   | 1:92:A:VAL:HB    | 15       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1402) | 1:112:A:VAL:HA   | 1:90:A:TYR:HE1   | 20       | 0.13          |
| (1,1392) | 1:126:A:VAL:HG21 | 1:90:A:TYR:HD1   | 2        | 0.13          |
| (1,1383) | 1:80:A:ALA:HB2   | 1:83:A:ILE:HG13  | 9        | 0.13          |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG11 | 5        | 0.13          |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG12 | 5        | 0.13          |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG13 | 5        | 0.13          |
| (1,412)  | 1:100:A:GLN:H    | 1:122:A:LEU:HG   | 10       | 0.13          |
| (1,368)  | 1:122:A:LEU:H    | 1:116:A:LEU:HD21 | 14       | 0.13          |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3   | 9        | 0.13          |
| (1,359)  | 1:70:A:THR:H     | 1:69:A:LEU:HB3   | 17       | 0.13          |
| (1,326)  | 1:93:A:TYR:H     | 1:124:A:GLY:HA3  | 14       | 0.13          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD11 | 10       | 0.13          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD12 | 10       | 0.13          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD13 | 10       | 0.13          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 2        | 0.13          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 6        | 0.13          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 9        | 0.13          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 14       | 0.13          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 16       | 0.13          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 17       | 0.13          |
| (1,220)  | 1:82:A:SER:H     | 1:82:A:SER:HA    | 2        | 0.13          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 5        | 0.13          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 5        | 0.13          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 5        | 0.13          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG21 | 6        | 0.13          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG22 | 6        | 0.13          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG23 | 6        | 0.13          |
| (1,197)  | 1:162:A:LYS:H    | 1:162:A:LYS:HD3  | 11       | 0.13          |
| (1,190)  | 1:151:A:ILE:H    | 1:147:A:ILE:HG22 | 7        | 0.13          |
| (1,190)  | 1:151:A:ILE:H    | 1:147:A:ILE:HG21 | 10       | 0.13          |
| (1,148)  | 1:91:A:ALA:H     | 1:126:A:VAL:HB   | 1        | 0.13          |
| (1,148)  | 1:91:A:ALA:H     | 1:126:A:VAL:HB   | 14       | 0.13          |
| (1,147)  | 1:74:A:LEU:H     | 1:73:A:GLU:HG3   | 5        | 0.13          |
| (1,110)  | 1:116:A:LEU:H    | 1:116:A:LEU:HD22 | 1        | 0.13          |
| (1,85)   | 1:125:A:SER:H    | 1:76:A:PRO:HB3   | 3        | 0.13          |
| (1,65)   | 1:100:A:GLN:HE22 | 1:122:A:LEU:HD12 | 1        | 0.13          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 4        | 0.13          |
| (1,2826) | 1:143:A:TRP:HZ2  | 1:147:A:ILE:HD12 | 7        | 0.12          |
| (1,2788) | 1:90:A:TYR:HD1   | 1:126:A:VAL:HG22 | 19       | 0.12          |
| (1,2354) | 1:73:A:GLU:HG3   | 1:75:A:LEU:H     | 11       | 0.12          |
| (1,2092) | 1:144:A:LYS:HG3  | 1:148:A:GLU:HG2  | 20       | 0.12          |
| (1,2027) | 1:70:A:THR:HB    | 1:149:A:GLU:HB3  | 9        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1962) | 1:162:A:LYS:HE2  | 1:159:A:PRO:HA   | 10       | 0.12          |
| (1,1962) | 1:162:A:LYS:HE2  | 1:159:A:PRO:HA   | 20       | 0.12          |
| (1,1953) | 1:130:A:ILE:HG21 | 1:88:A:GLY:HA2   | 18       | 0.12          |
| (1,1902) | 1:77:A:ILE:HA    | 1:76:A:PRO:HB3   | 1        | 0.12          |
| (1,1902) | 1:77:A:ILE:HA    | 1:76:A:PRO:HB3   | 4        | 0.12          |
| (1,1902) | 1:77:A:ILE:HA    | 1:76:A:PRO:HB3   | 20       | 0.12          |
| (1,1901) | 1:85:A:SER:HB2   | 1:109:A:ALA:HB1  | 2        | 0.12          |
| (1,1897) | 1:85:A:SER:HB2   | 1:84:A:PRO:HA    | 4        | 0.12          |
| (1,1897) | 1:85:A:SER:HB2   | 1:84:A:PRO:HA    | 12       | 0.12          |
| (1,1881) | 1:169:A:VAL:HG21 | 1:168:A:PHE:H    | 19       | 0.12          |
| (1,1863) | 1:95:A:LYS:HE3   | 1:95:A:LYS:H     | 17       | 0.12          |
| (1,1844) | 1:108:A:ILE:HA   | 1:110:A:ALA:HB3  | 6        | 0.12          |
| (1,1834) | 1:147:A:ILE:HD12 | 1:143:A:TRP:HZ2  | 7        | 0.12          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG21 | 5        | 0.12          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG22 | 5        | 0.12          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG23 | 5        | 0.12          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG21 | 9        | 0.12          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG22 | 9        | 0.12          |
| (1,1793) | 1:144:A:LYS:HD2  | 1:147:A:ILE:HG23 | 9        | 0.12          |
| (1,1761) | 1:170:A:LYS:HD2  | 1:170:A:LYS:H    | 19       | 0.12          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG21 | 3        | 0.12          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG22 | 3        | 0.12          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG23 | 3        | 0.12          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG21 | 3        | 0.12          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG22 | 3        | 0.12          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG23 | 3        | 0.12          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG21 | 3        | 0.12          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG22 | 3        | 0.12          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG23 | 3        | 0.12          |
| (1,1690) | 1:145:A:LEU:HD21 | 1:67:A:LYS:H     | 6        | 0.12          |
| (1,1690) | 1:145:A:LEU:HD22 | 1:67:A:LYS:H     | 6        | 0.12          |
| (1,1690) | 1:145:A:LEU:HD23 | 1:67:A:LYS:H     | 6        | 0.12          |
| (1,1659) | 1:104:A:ILE:HG21 | 1:143:A:TRP:HB3  | 1        | 0.12          |
| (1,1659) | 1:104:A:ILE:HG23 | 1:143:A:TRP:HA   | 3        | 0.12          |
| (1,1659) | 1:104:A:ILE:HG22 | 1:143:A:TRP:HA   | 20       | 0.12          |
| (1,1645) | 1:108:A:ILE:HG23 | 1:84:A:PRO:HD2   | 11       | 0.12          |
| (1,1582) | 1:102:A:VAL:HB   | 1:147:A:ILE:HG22 | 15       | 0.12          |
| (1,1579) | 1:76:A:PRO:HB2   | 1:77:A:ILE:HG22  | 10       | 0.12          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 2        | 0.12          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 8        | 0.12          |
| (1,1562) | 1:125:A:SER:HB3  | 1:74:A:LEU:HB2   | 20       | 0.12          |
| (1,1555) | 1:148:A:GLU:HG3  | 1:147:A:ILE:HG21 | 16       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1539) | 1:69:A:LEU:HD11  | 1:150:A:HIS:HA   | 2        | 0.12          |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG11 | 11       | 0.12          |
| (1,1523) | 1:156:A:LYS:HB3  | 1:157:A:VAL:HG21 | 19       | 0.12          |
| (1,1511) | 1:128:A:VAL:HG12 | 1:90:A:TYR:H     | 4        | 0.12          |
| (1,1503) | 1:80:A:ALA:HA    | 1:83:A:ILE:HD11  | 7        | 0.12          |
| (1,1487) | 1:126:A:VAL:HA   | 1:92:A:VAL:HB    | 7        | 0.12          |
| (1,1487) | 1:126:A:VAL:HA   | 1:75:A:LEU:HB2   | 8        | 0.12          |
| (1,1487) | 1:126:A:VAL:HA   | 1:92:A:VAL:HB    | 19       | 0.12          |
| (1,1470) | 1:159:A:PRO:HD3  | 1:162:A:LYS:HG3  | 1        | 0.12          |
| (1,1464) | 1:152:A:LYS:HA   | 1:152:A:LYS:HG3  | 2        | 0.12          |
| (1,1402) | 1:112:A:VAL:HA   | 1:115:A:HIS:HD2  | 15       | 0.12          |
| (1,1392) | 1:126:A:VAL:HG22 | 1:90:A:TYR:HD1   | 19       | 0.12          |
| (1,1228) | 1:169:A:VAL:H    | 1:168:A:PHE:HD1  | 8        | 0.12          |
| (1,1098) | 1:148:A:GLU:H    | 1:144:A:LYS:HG3  | 2        | 0.12          |
| (1,1042) | 1:100:A:GLN:H    | 1:150:A:HIS:HB3  | 9        | 0.12          |
| (1,410)  | 1:95:A:LYS:H     | 1:95:A:LYS:HE3   | 17       | 0.12          |
| (1,396)  | 1:100:A:GLN:H    | 1:98:A:GLU:HB3   | 18       | 0.12          |
| (1,356)  | 1:100:A:GLN:H    | 1:102:A:VAL:HG12 | 17       | 0.12          |
| (1,302)  | 1:146:A:TRP:HE1  | 1:69:A:LEU:HB3   | 19       | 0.12          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD21 | 6        | 0.12          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD22 | 6        | 0.12          |
| (1,281)  | 1:67:A:LYS:H     | 1:145:A:LEU:HD23 | 6        | 0.12          |
| (1,277)  | 1:67:A:LYS:H     | 1:146:A:TRP:HZ2  | 7        | 0.12          |
| (1,260)  | 1:128:A:VAL:H    | 1:91:A:ALA:HB2   | 19       | 0.12          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 4        | 0.12          |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 12       | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 3        | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 3        | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 3        | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 12       | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 12       | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 12       | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG11 | 15       | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG12 | 15       | 0.12          |
| (1,203)  | 1:129:A:GLY:H    | 1:128:A:VAL:HG13 | 15       | 0.12          |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 1        | 0.12          |
| (1,148)  | 1:91:A:ALA:H     | 1:126:A:VAL:HB   | 12       | 0.12          |
| (1,101)  | 1:89:A:VAL:H     | 1:131:A:VAL:HG11 | 15       | 0.12          |
| (1,95)   | 1:153:A:VAL:H    | 1:153:A:VAL:HB   | 5        | 0.12          |
| (1,93)   | 1:114:A:ALA:H    | 1:113:A:SER:HB2  | 11       | 0.12          |
| (1,75)   | 1:141:A:GLN:HE21 | 1:145:A:LEU:HB2  | 3        | 0.12          |
| (1,57)   | 1:101:A:PHE:H    | 1:100:A:GLN:HE21 | 14       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,44)   | 1:160:A:GLY:H    | 1:159:A:PRO:HB2  | 9        | 0.12          |
| (1,2799) | 1:93:A:TYR:HE2   | 1:69:A:LEU:HD12  | 7        | 0.11          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB3   | 12       | 0.11          |
| (1,2795) | 1:93:A:TYR:HD1   | 1:91:A:ALA:HB3   | 16       | 0.11          |
| (1,2711) | 1:89:A:VAL:HB    | 1:104:A:ILE:HD11 | 19       | 0.11          |
| (1,2711) | 1:89:A:VAL:HB    | 1:104:A:ILE:HD12 | 19       | 0.11          |
| (1,2711) | 1:89:A:VAL:HB    | 1:104:A:ILE:HD13 | 19       | 0.11          |
| (1,2656) | 1:86:A:ALA:HB1   | 1:107:A:ASN:HD21 | 6        | 0.11          |
| (1,2656) | 1:86:A:ALA:HB2   | 1:107:A:ASN:HD21 | 6        | 0.11          |
| (1,2656) | 1:86:A:ALA:HB3   | 1:107:A:ASN:HD21 | 6        | 0.11          |
| (1,2656) | 1:86:A:ALA:HB1   | 1:107:A:ASN:HD21 | 17       | 0.11          |
| (1,2656) | 1:86:A:ALA:HB2   | 1:107:A:ASN:HD21 | 17       | 0.11          |
| (1,2656) | 1:86:A:ALA:HB3   | 1:107:A:ASN:HD21 | 17       | 0.11          |
| (1,1962) | 1:162:A:LYS:HE2  | 1:159:A:PRO:HA   | 4        | 0.11          |
| (1,1946) | 1:68:A:SER:HB2   | 1:146:A:TRP:H    | 10       | 0.11          |
| (1,1823) | 1:87:A:SER:HB3   | 1:86:A:ALA:HB2   | 13       | 0.11          |
| (1,1777) | 1:162:A:LYS:HD3  | 1:162:A:LYS:H    | 13       | 0.11          |
| (1,1751) | 1:108:A:ILE:HG21 | 1:111:A:SER:H    | 18       | 0.11          |
| (1,1724) | 1:122:A:LEU:HD13 | 1:101:A:PHE:H    | 1        | 0.11          |
| (1,1724) | 1:122:A:LEU:HD13 | 1:101:A:PHE:H    | 10       | 0.11          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG21 | 4        | 0.11          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG22 | 4        | 0.11          |
| (1,1691) | 1:72:A:THR:HG21  | 1:128:A:VAL:HG23 | 4        | 0.11          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG21 | 4        | 0.11          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG22 | 4        | 0.11          |
| (1,1691) | 1:72:A:THR:HG22  | 1:128:A:VAL:HG23 | 4        | 0.11          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG21 | 4        | 0.11          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG22 | 4        | 0.11          |
| (1,1691) | 1:72:A:THR:HG23  | 1:128:A:VAL:HG23 | 4        | 0.11          |
| (1,1616) | 1:66:A:VAL:HG21  | 1:131:A:VAL:HB   | 6        | 0.11          |
| (1,1616) | 1:66:A:VAL:HG22  | 1:131:A:VAL:HB   | 6        | 0.11          |
| (1,1616) | 1:66:A:VAL:HG23  | 1:131:A:VAL:HB   | 6        | 0.11          |
| (1,1566) | 1:119:A:VAL:HG23 | 1:167:A:THR:HG22 | 4        | 0.11          |
| (1,1512) | 1:73:A:GLU:HG2   | 1:72:A:THR:HG23  | 5        | 0.11          |
| (1,1511) | 1:128:A:VAL:HG11 | 1:90:A:TYR:H     | 3        | 0.11          |
| (1,1506) | 1:170:A:LYS:HE2  | 1:171:A:VAL:H    | 16       | 0.11          |
| (1,1502) | 1:84:A:PRO:HG2   | 1:75:A:LEU:HD23  | 13       | 0.11          |
| (1,1042) | 1:100:A:GLN:H    | 1:150:A:HIS:HB3  | 8        | 0.11          |
| (1,948)  | 1:102:A:VAL:H    | 1:160:A:GLY:HA3  | 15       | 0.11          |
| (1,864)  | 1:86:A:ALA:H     | 1:107:A:ASN:HD21 | 1        | 0.11          |
| (1,462)  | 1:95:A:LYS:H     | 1:95:A:LYS:HG2   | 18       | 0.11          |
| (1,373)  | 1:147:A:ILE:H    | 1:102:A:VAL:HG11 | 20       | 0.11          |

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| Key     | Atom-1        | Atom-2           | Model ID | Violation (Å) |
|---------|---------------|------------------|----------|---------------|
| (1,343) | 1:96:A:SER:H  | 1:95:A:LYS:HD3   | 14       | 0.11          |
| (1,337) | 1:93:A:TYR:H  | 1:77:A:ILE:HD13  | 5        | 0.11          |
| (1,337) | 1:93:A:TYR:H  | 1:77:A:ILE:HD13  | 7        | 0.11          |
| (1,337) | 1:93:A:TYR:H  | 1:77:A:ILE:HD11  | 8        | 0.11          |
| (1,337) | 1:93:A:TYR:H  | 1:77:A:ILE:HD12  | 11       | 0.11          |
| (1,309) | 1:88:A:GLY:H  | 1:87:A:SER:HB3   | 15       | 0.11          |
| (1,295) | 1:108:A:ILE:H | 1:87:A:SER:HB2   | 18       | 0.11          |
| (1,285) | 1:108:A:ILE:H | 1:83:A:ILE:HG23  | 6        | 0.11          |
| (1,275) | 1:150:A:HIS:H | 1:149:A:GLU:HB2  | 2        | 0.11          |
| (1,256) | 1:68:A:SER:H  | 1:68:A:SER:HA    | 3        | 0.11          |
| (1,220) | 1:82:A:SER:H  | 1:82:A:SER:HA    | 1        | 0.11          |
| (1,220) | 1:82:A:SER:H  | 1:82:A:SER:HA    | 3        | 0.11          |
| (1,220) | 1:82:A:SER:H  | 1:82:A:SER:HA    | 4        | 0.11          |
| (1,220) | 1:82:A:SER:H  | 1:82:A:SER:HA    | 9        | 0.11          |
| (1,220) | 1:82:A:SER:H  | 1:82:A:SER:HA    | 15       | 0.11          |
| (1,220) | 1:82:A:SER:H  | 1:82:A:SER:HA    | 18       | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG21 | 4        | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG22 | 4        | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG23 | 4        | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG11 | 10       | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG12 | 10       | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG13 | 10       | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG11 | 16       | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG12 | 16       | 0.11          |
| (1,203) | 1:129:A:GLY:H | 1:128:A:VAL:HG13 | 16       | 0.11          |
| (1,197) | 1:162:A:LYS:H | 1:162:A:LYS:HD3  | 13       | 0.11          |
| (1,184) | 1:149:A:GLU:H | 1:145:A:LEU:HD21 | 7        | 0.11          |
| (1,184) | 1:149:A:GLU:H | 1:145:A:LEU:HD22 | 7        | 0.11          |
| (1,184) | 1:149:A:GLU:H | 1:145:A:LEU:HD23 | 7        | 0.11          |
| (1,163) | 1:112:A:VAL:H | 1:108:A:ILE:HB   | 12       | 0.11          |
| (1,150) | 1:142:A:ALA:H | 1:145:A:LEU:HB2  | 2        | 0.11          |
| (1,150) | 1:142:A:ALA:H | 1:145:A:LEU:HB2  | 5        | 0.11          |
| (1,150) | 1:142:A:ALA:H | 1:145:A:LEU:HB2  | 19       | 0.11          |
| (1,148) | 1:91:A:ALA:H  | 1:128:A:VAL:HB   | 4        | 0.11          |
| (1,110) | 1:116:A:LEU:H | 1:116:A:LEU:HD23 | 5        | 0.11          |
| (1,110) | 1:116:A:LEU:H | 1:116:A:LEU:HD22 | 13       | 0.11          |
| (1,99)  | 1:160:A:GLY:H | 1:122:A:LEU:HD13 | 14       | 0.11          |
| (1,85)  | 1:125:A:SER:H | 1:76:A:PRO:HB3   | 16       | 0.11          |
| (1,80)  | 1:144:A:LYS:H | 1:143:A:TRP:HB2  | 13       | 0.11          |
| (1,66)  | 1:123:A:CYS:H | 1:116:A:LEU:HD22 | 19       | 0.11          |
| (1,44)  | 1:160:A:GLY:H | 1:159:A:PRO:HB2  | 12       | 0.11          |
| (1,44)  | 1:160:A:GLY:H | 1:159:A:PRO:HB2  | 13       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,44)   | 1:160:A:GLY:H    | 1:159:A:PRO:HB2  | 14       | 0.11          |
| (1,37)   | 1:88:A:GLY:H     | 1:108:A:ILE:HB   | 3        | 0.11          |
| (1,4)    | 1:142:A:ALA:H    | 1:145:A:LEU:HB2  | 2        | 0.11          |
| (1,2656) | 1:86:A:ALA:HB1   | 1:107:A:ASN:HD21 | 3        | 0.1           |
| (1,2656) | 1:86:A:ALA:HB2   | 1:107:A:ASN:HD21 | 3        | 0.1           |
| (1,2656) | 1:86:A:ALA:HB3   | 1:107:A:ASN:HD21 | 3        | 0.1           |
| (1,2656) | 1:86:A:ALA:HB1   | 1:107:A:ASN:HD21 | 7        | 0.1           |
| (1,2656) | 1:86:A:ALA:HB2   | 1:107:A:ASN:HD21 | 7        | 0.1           |
| (1,2656) | 1:86:A:ALA:HB3   | 1:107:A:ASN:HD21 | 7        | 0.1           |
| (1,1983) | 1:77:A:ILE:HD13  | 1:125:A:SER:H    | 6        | 0.1           |
| (1,1962) | 1:162:A:LYS:HE2  | 1:159:A:PRO:HA   | 7        | 0.1           |
| (1,1915) | 1:120:A:PRO:HA   | 1:116:A:LEU:HD23 | 16       | 0.1           |
| (1,1904) | 1:100:A:GLN:HA   | 1:156:A:LYS:HG2  | 1        | 0.1           |
| (1,1751) | 1:108:A:ILE:HG23 | 1:111:A:SER:H    | 4        | 0.1           |
| (1,1741) | 1:157:A:VAL:HG11 | 1:143:A:TRP:HH2  | 1        | 0.1           |
| (1,1741) | 1:157:A:VAL:HG12 | 1:143:A:TRP:HH2  | 1        | 0.1           |
| (1,1741) | 1:157:A:VAL:HG13 | 1:143:A:TRP:HH2  | 1        | 0.1           |
| (1,1727) | 1:145:A:LEU:HD21 | 1:141:A:GLN:HB3  | 20       | 0.1           |
| (1,1727) | 1:145:A:LEU:HD22 | 1:141:A:GLN:HB3  | 20       | 0.1           |
| (1,1727) | 1:145:A:LEU:HD23 | 1:141:A:GLN:HB3  | 20       | 0.1           |
| (1,1710) | 1:156:A:LYS:HG2  | 1:100:A:GLN:HA   | 1        | 0.1           |
| (1,1683) | 1:144:A:LYS:HG2  | 1:147:A:ILE:HG22 | 18       | 0.1           |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD11  | 13       | 0.1           |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD12  | 13       | 0.1           |
| (1,1681) | 1:156:A:LYS:HG3  | 1:99:A:LEU:HD13  | 13       | 0.1           |
| (1,1640) | 1:159:A:PRO:HB3  | 1:162:A:LYS:HE2  | 10       | 0.1           |
| (1,1487) | 1:126:A:VAL:HA   | 1:92:A:VAL:HB    | 3        | 0.1           |
| (1,948)  | 1:102:A:VAL:H    | 1:160:A:GLY:HA3  | 17       | 0.1           |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG11 | 17       | 0.1           |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG12 | 17       | 0.1           |
| (1,743)  | 1:123:A:CYS:H    | 1:119:A:VAL:HG13 | 17       | 0.1           |
| (1,256)  | 1:68:A:SER:H     | 1:68:A:SER:HA    | 15       | 0.1           |
| (1,240)  | 1:94:A:ASP:H     | 1:100:A:GLN:HG2  | 12       | 0.1           |
| (1,230)  | 1:115:A:HIS:H    | 1:115:A:HIS:HB2  | 3        | 0.1           |
| (1,220)  | 1:82:A:SER:H     | 1:82:A:SER:HA    | 11       | 0.1           |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 13       | 0.1           |
| (1,163)  | 1:112:A:VAL:H    | 1:108:A:ILE:HB   | 19       | 0.1           |
| (1,90)   | 1:124:A:GLY:H    | 1:77:A:ILE:HG13  | 5        | 0.1           |
| (1,44)   | 1:160:A:GLY:H    | 1:159:A:PRO:HB2  | 16       | 0.1           |
| (1,7)    | 1:139:A:LEU:H    | 1:138:A:VAL:HG11 | 8        | 0.1           |

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

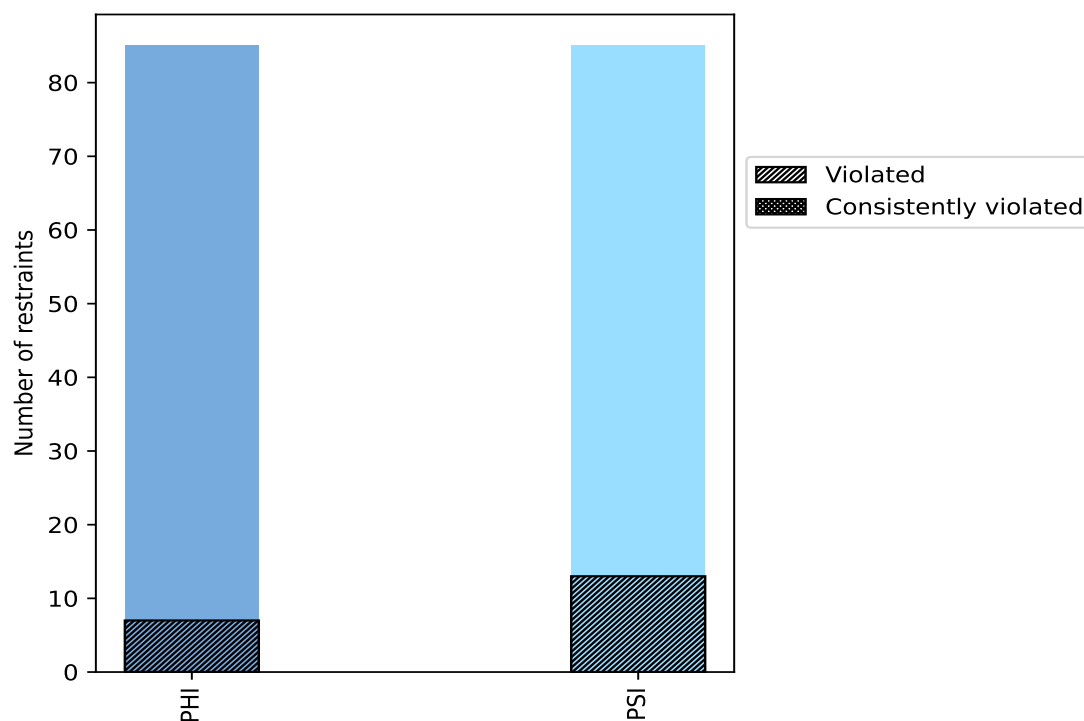
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 85    | 50.0           | 7                     | 8.2            | 4.1            | 0                                  | 0.0            | 0.0            |
| PSI        | 85    | 50.0           | 13                    | 15.3           | 7.6            | 0                                  | 0.0            | 0.0            |
| Total      | 170   | 100.0          | 20                    | 11.8           | 11.8           | 0                                  | 0.0            | 0.0            |

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

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



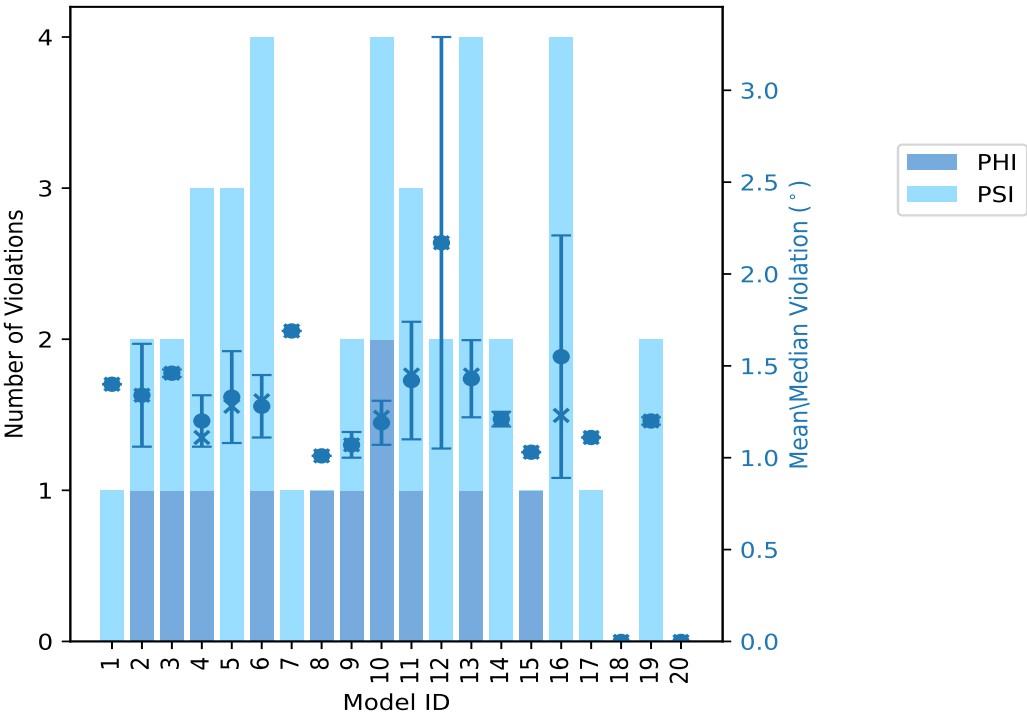
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 0                    | 1   | 1     | 1.4      | 1.4     | 0.0    | 1.4        |
| 2        | 1                    | 1   | 2     | 1.34     | 1.61    | 0.28   | 1.34       |
| 3        | 1                    | 1   | 2     | 1.46     | 1.48    | 0.02   | 1.46       |
| 4        | 1                    | 2   | 3     | 1.2      | 1.4     | 0.14   | 1.11       |
| 5        | 0                    | 3   | 3     | 1.33     | 1.66    | 0.25   | 1.28       |
| 6        | 1                    | 3   | 4     | 1.28     | 1.48    | 0.17   | 1.31       |
| 7        | 0                    | 1   | 1     | 1.69     | 1.69    | 0.0    | 1.69       |
| 8        | 1                    | 0   | 1     | 1.01     | 1.01    | 0.0    | 1.01       |
| 9        | 1                    | 1   | 2     | 1.07     | 1.14    | 0.07   | 1.07       |
| 10       | 2                    | 2   | 4     | 1.19     | 1.33    | 0.12   | 1.22       |
| 11       | 1                    | 2   | 3     | 1.42     | 1.8     | 0.32   | 1.45       |
| 12       | 0                    | 2   | 2     | 2.17     | 3.29    | 1.12   | 2.17       |
| 13       | 1                    | 3   | 4     | 1.43     | 1.69    | 0.21   | 1.45       |
| 14       | 0                    | 2   | 2     | 1.21     | 1.25    | 0.04   | 1.21       |
| 15       | 1                    | 0   | 1     | 1.03     | 1.03    | 0.0    | 1.03       |
| 16       | 0                    | 4   | 4     | 1.55     | 2.68    | 0.66   | 1.23       |
| 17       | 0                    | 1   | 1     | 1.11     | 1.11    | 0.0    | 1.11       |
| 18       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 19       | 0                    | 2   | 2     | 1.2      | 1.22    | 0.02   | 1.2        |
| 20       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

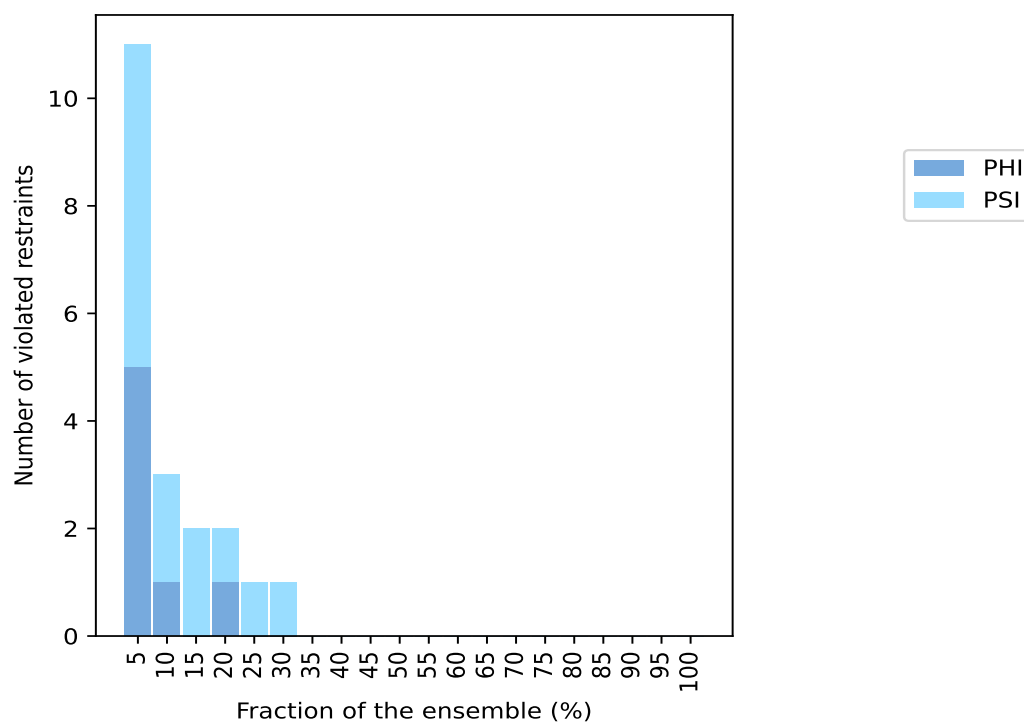
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |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

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

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

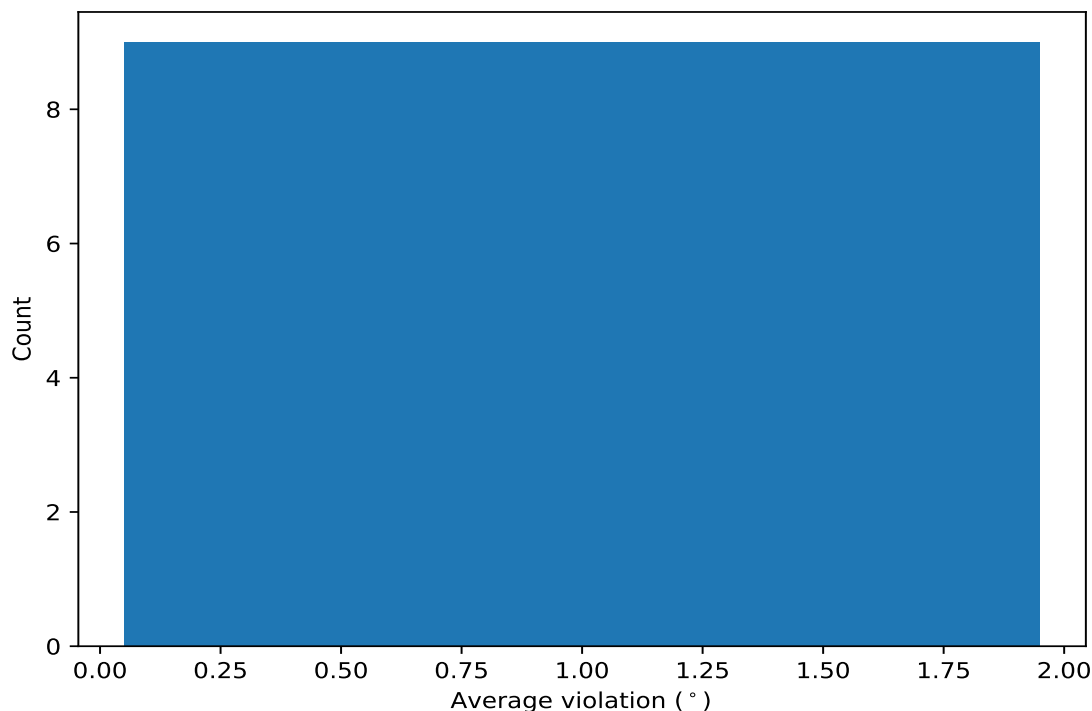


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

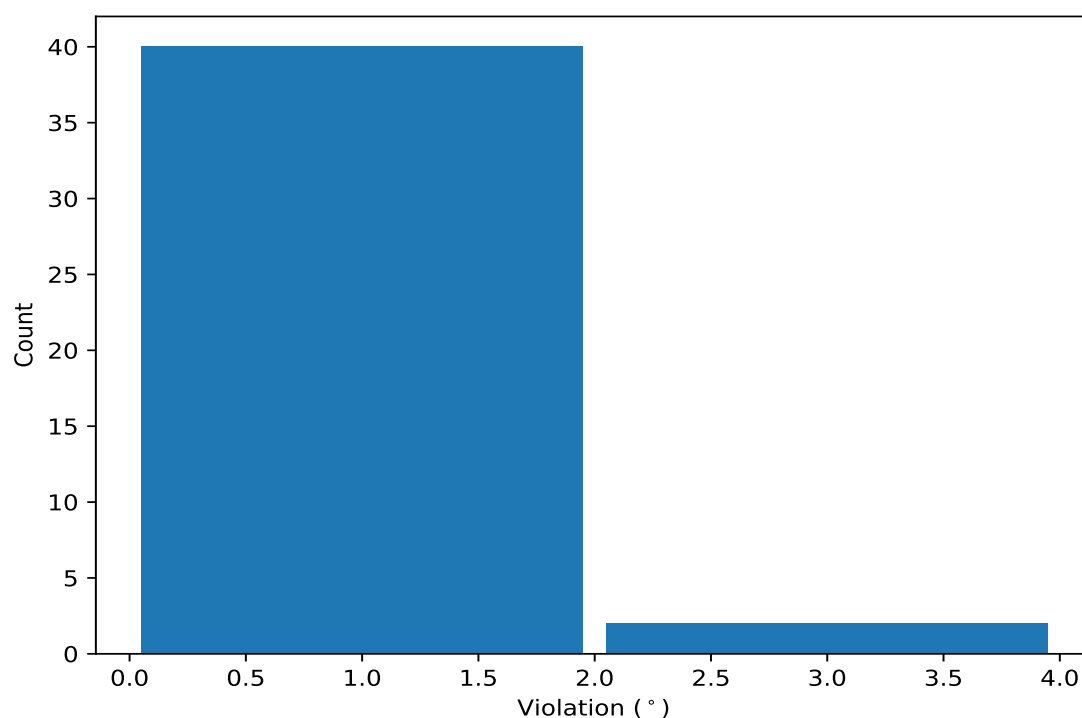
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,22)  | 1:79:A:GLU:N  | 1:79:A:GLU:CA  | 1:79:A:GLU:C   | 1:80:A:ALA:N  | 6                   | 1.88 | 0.81            | 1.42   |
| (1,160) | 1:165:A:ASN:N | 1:165:A:ASN:CA | 1:165:A:ASN:C  | 1:166:A:ASN:N | 5                   | 1.12 | 0.08            | 1.14   |
| (1,57)  | 1:100:A:GLN:C | 1:101:A:PHE:N  | 1:101:A:PHE:CA | 1:101:A:PHE:C | 4                   | 1.47 | 0.29            | 1.53   |
| (1,56)  | 1:100:A:GLN:N | 1:100:A:GLN:CA | 1:100:A:GLN:C  | 1:101:A:PHE:N | 4                   | 1.33 | 0.24            | 1.29   |
| (1,94)  | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:CYS:N | 3                   | 1.31 | 0.18            | 1.19   |
| (1,32)  | 1:84:A:PRO:N  | 1:84:A:PRO:CA  | 1:84:A:PRO:C   | 1:85:A:SER:N  | 3                   | 1.17 | 0.08            | 1.14   |
| (1,166) | 1:169:A:VAL:N | 1:169:A:VAL:CA | 1:169:A:VAL:C  | 1:170:A:LYS:N | 2                   | 1.46 | 0.24            | 1.46   |
| (1,150) | 1:154:A:THR:N | 1:154:A:THR:CA | 1:154:A:THR:C  | 1:155:A:GLY:N | 2                   | 1.4  | 0.08            | 1.4    |
| (1,163) | 1:167:A:THR:C | 1:168:A:PHE:N  | 1:168:A:PHE:CA | 1:168:A:PHE:C | 2                   | 1.06 | 0.05            | 1.06   |

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

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

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

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,22)  | 1:79:A:GLU:N  | 1:79:A:GLU:CA  | 1:79:A:GLU:C   | 1:80:A:ALA:N  | 12       | 3.29          |
| (1,22)  | 1:79:A:GLU:N  | 1:79:A:GLU:CA  | 1:79:A:GLU:C   | 1:80:A:ALA:N  | 16       | 2.68          |
| (1,57)  | 1:100:A:GLN:C | 1:101:A:PHE:N  | 1:101:A:PHE:CA | 1:101:A:PHE:C | 11       | 1.8           |
| (1,166) | 1:169:A:VAL:N | 1:169:A:VAL:CA | 1:169:A:VAL:C  | 1:170:A:LYS:N | 13       | 1.69          |
| (1,56)  | 1:100:A:GLN:N | 1:100:A:GLN:CA | 1:100:A:GLN:C  | 1:101:A:PHE:N | 7        | 1.69          |
| (1,92)  | 1:121:A:GLU:N | 1:121:A:GLU:CA | 1:121:A:GLU:C  | 1:122:A:LEU:N | 5        | 1.66          |
| (1,57)  | 1:100:A:GLN:C | 1:101:A:PHE:N  | 1:101:A:PHE:CA | 1:101:A:PHE:C | 2        | 1.61          |
| (1,94)  | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:CYS:N | 13       | 1.57          |
| (1,150) | 1:154:A:THR:N | 1:154:A:THR:CA | 1:154:A:THR:C  | 1:155:A:GLY:N | 3        | 1.48          |
| (1,20)  | 1:78:A:THR:N  | 1:78:A:THR:CA  | 1:78:A:THR:C   | 1:79:A:GLU:N  | 6        | 1.48          |
| (1,57)  | 1:100:A:GLN:C | 1:101:A:PHE:N  | 1:101:A:PHE:CA | 1:101:A:PHE:C | 3        | 1.45          |
| (1,22)  | 1:79:A:GLU:N  | 1:79:A:GLU:CA  | 1:79:A:GLU:C   | 1:80:A:ALA:N  | 11       | 1.45          |
| (1,56)  | 1:100:A:GLN:N | 1:100:A:GLN:CA | 1:100:A:GLN:C  | 1:101:A:PHE:N | 4        | 1.4           |
| (1,22)  | 1:79:A:GLU:N  | 1:79:A:GLU:CA  | 1:79:A:GLU:C   | 1:80:A:ALA:N  | 1        | 1.4           |
| (1,167) | 1:175:A:HIS:C | 1:176:A:HIS:N  | 1:176:A:HIS:CA | 1:176:A:HIS:C | 10       | 1.33          |
| (1,99)  | 1:126:A:VAL:C | 1:127:A:LYS:N  | 1:127:A:LYS:CA | 1:127:A:LYS:C | 13       | 1.33          |
| (1,22)  | 1:79:A:GLU:N  | 1:79:A:GLU:CA  | 1:79:A:GLU:C   | 1:80:A:ALA:N  | 6        | 1.33          |
| (1,150) | 1:154:A:THR:N | 1:154:A:THR:CA | 1:154:A:THR:C  | 1:155:A:GLY:N | 16       | 1.31          |
| (1,32)  | 1:84:A:PRO:N  | 1:84:A:PRO:CA  | 1:84:A:PRO:C   | 1:85:A:SER:N  | 6        | 1.29          |
| (1,156) | 1:159:A:PRO:N | 1:159:A:PRO:CA | 1:159:A:PRO:C  | 1:160:A:GLY:N | 5        | 1.28          |
| (1,160) | 1:165:A:ASN:N | 1:165:A:ASN:CA | 1:165:A:ASN:C  | 1:166:A:ASN:N | 14       | 1.25          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,33)  | 1:85:A:SER:C  | 1:86:A:ALA:N   | 1:86:A:ALA:CA  | 1:86:A:ALA:C  | 10       | 1.25          |
| (1,166) | 1:169:A:VAL:N | 1:169:A:VAL:CA | 1:169:A:VAL:C  | 1:170:A:LYS:N | 19       | 1.22          |
| (1,94)  | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:CYS:N | 10       | 1.19          |
| (1,94)  | 1:122:A:LEU:N | 1:122:A:LEU:CA | 1:122:A:LEU:C  | 1:123:A:CYS:N | 14       | 1.18          |
| (1,56)  | 1:100:A:GLN:N | 1:100:A:GLN:CA | 1:100:A:GLN:C  | 1:101:A:PHE:N | 19       | 1.18          |
| (1,160) | 1:165:A:ASN:N | 1:165:A:ASN:CA | 1:165:A:ASN:C  | 1:166:A:ASN:N | 16       | 1.16          |
| (1,160) | 1:165:A:ASN:N | 1:165:A:ASN:CA | 1:165:A:ASN:C  | 1:166:A:ASN:N | 9        | 1.14          |
| (1,32)  | 1:84:A:PRO:N  | 1:84:A:PRO:CA  | 1:84:A:PRO:C   | 1:85:A:SER:N  | 13       | 1.14          |
| (1,163) | 1:167:A:THR:C | 1:168:A:PHE:N  | 1:168:A:PHE:CA | 1:168:A:PHE:C | 4        | 1.11          |
| (1,22)  | 1:79:A:GLU:N  | 1:79:A:GLU:CA  | 1:79:A:GLU:C   | 1:80:A:ALA:N  | 17       | 1.11          |
| (1,32)  | 1:84:A:PRO:N  | 1:84:A:PRO:CA  | 1:84:A:PRO:C   | 1:85:A:SER:N  | 4        | 1.09          |
| (1,152) | 1:155:A:GLY:N | 1:155:A:GLY:CA | 1:155:A:GLY:C  | 1:156:A:LYS:N | 2        | 1.06          |
| (1,56)  | 1:100:A:GLN:N | 1:100:A:GLN:CA | 1:100:A:GLN:C  | 1:101:A:PHE:N | 5        | 1.06          |
| (1,168) | 1:176:A:HIS:N | 1:176:A:HIS:CA | 1:176:A:HIS:C  | 1:177:A:HIS:N | 16       | 1.05          |
| (1,160) | 1:165:A:ASN:N | 1:165:A:ASN:CA | 1:165:A:ASN:C  | 1:166:A:ASN:N | 12       | 1.05          |
| (1,9)   | 1:71:A:GLU:C  | 1:72:A:THR:N   | 1:72:A:THR:CA  | 1:72:A:THR:C  | 15       | 1.03          |
| (1,57)  | 1:100:A:GLN:C | 1:101:A:PHE:N  | 1:101:A:PHE:CA | 1:101:A:PHE:C | 6        | 1.02          |
| (1,163) | 1:167:A:THR:C | 1:168:A:PHE:N  | 1:168:A:PHE:CA | 1:168:A:PHE:C | 8        | 1.01          |
| (1,160) | 1:165:A:ASN:N | 1:165:A:ASN:CA | 1:165:A:ASN:C  | 1:166:A:ASN:N | 11       | 1.01          |
| (1,34)  | 1:86:A:ALA:N  | 1:86:A:ALA:CA  | 1:86:A:ALA:C   | 1:87:A:SER:N  | 10       | 1.01          |
| (1,55)  | 1:99:A:LEU:C  | 1:100:A:GLN:N  | 1:100:A:GLN:CA | 1:100:A:GLN:C | 9        | 1.0           |