



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 08:07 AM UTC

PDB ID : 2M3E / pdb\_00002m3e  
BMRB ID : 18958  
Title : The Integrin Alpha L Transmembrane Domain in Bicelles: Structure and Interaction with Integrin Beta 2  
Authors : Surya, W.; Li, Y.; Millet, O.; Diercks, T.; Torres, J.  
Deposited on : 2013-01-17

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
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

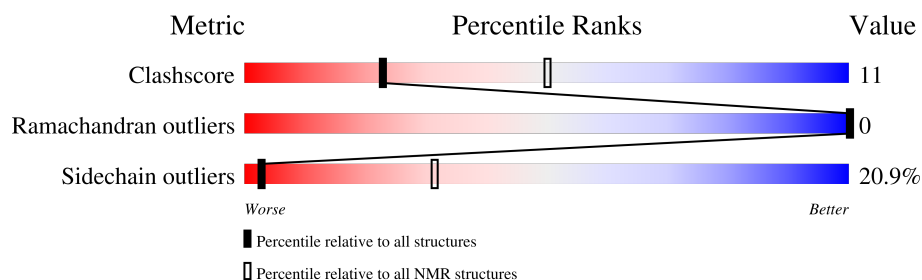
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 86%.

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     | 50     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1065-A:1089 (25)    | 0.11              | 7            |

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 837 atoms, of which 435 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Integrin alpha-L.

| Mol | Chain | Residues | Atoms |     |     |    |    |   |  | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|--|-------|
| 1   | A     | 50       | Total | C   | H   | N  | O  | S |  | 0     |
|     |       |          | 837   | 272 | 435 | 61 | 67 | 2 |  |       |

There are 3 discrepancies between the modelled and reference sequences:

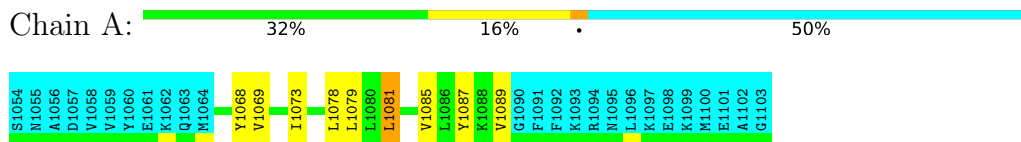
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1054    | SER      | -      | expression tag | UNP P20701 |
| A     | 1055    | ASN      | -      | expression tag | UNP P20701 |
| A     | 1056    | ALA      | -      | expression tag | UNP P20701 |

## 4 Residue-property plots [i](#)

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

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

- Molecule 1: Integrin alpha-L

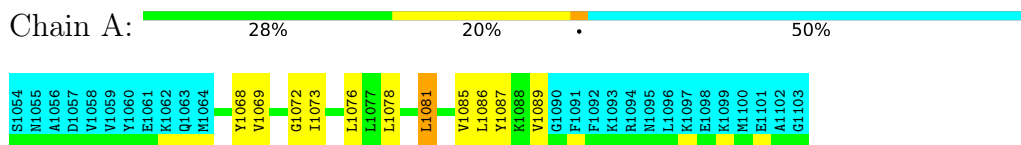


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

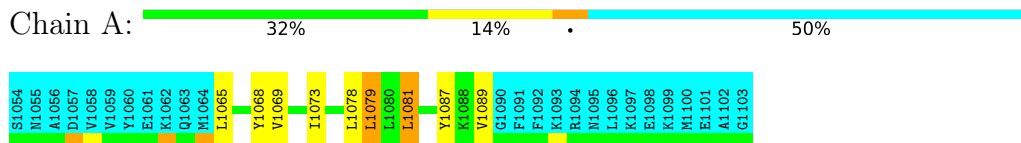
#### 4.2.1 Score per residue for model 1

- Molecule 1: Integrin alpha-L



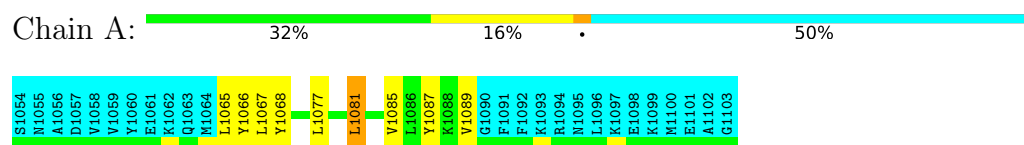
#### 4.2.2 Score per residue for model 2

- Molecule 1: Integrin alpha-L



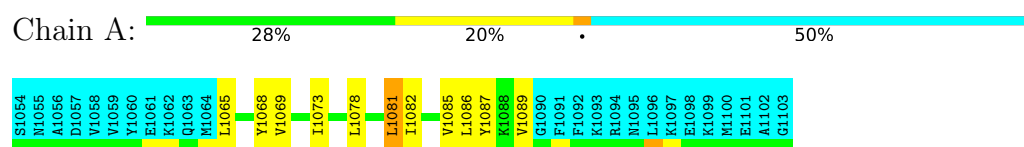
### 4.2.3 Score per residue for model 3

- Molecule 1: Integrin alpha-L



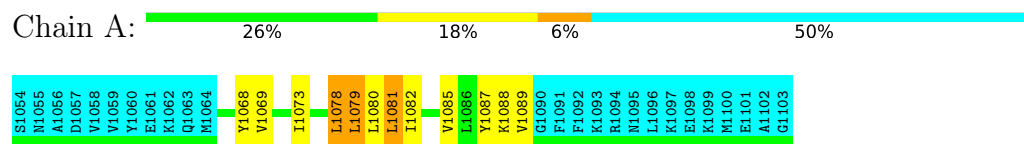
### 4.2.4 Score per residue for model 4

- Molecule 1: Integrin alpha-L



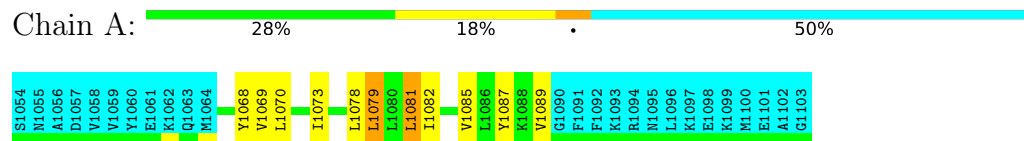
### 4.2.5 Score per residue for model 5

- Molecule 1: Integrin alpha-L



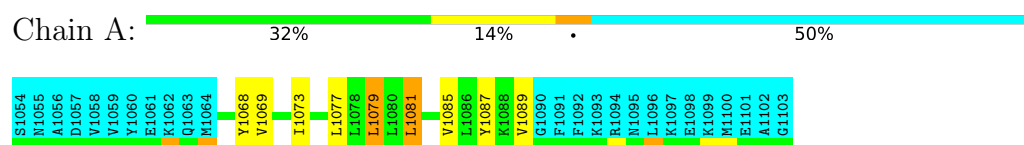
### 4.2.6 Score per residue for model 6

- Molecule 1: Integrin alpha-L



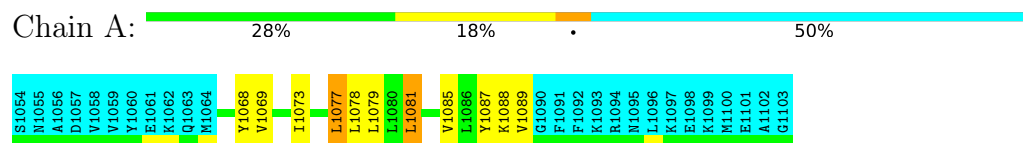
### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Integrin alpha-L



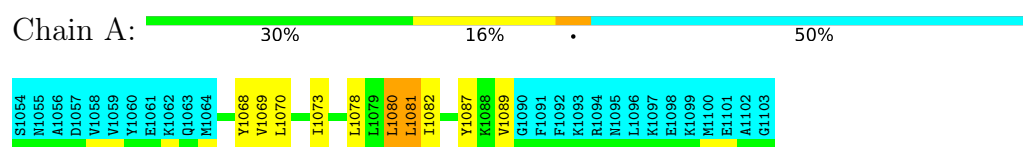
### 4.2.8 Score per residue for model 8

- Molecule 1: Integrin alpha-L



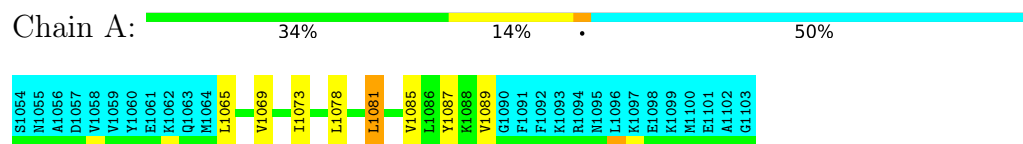
### 4.2.9 Score per residue for model 9

- Molecule 1: Integrin alpha-L



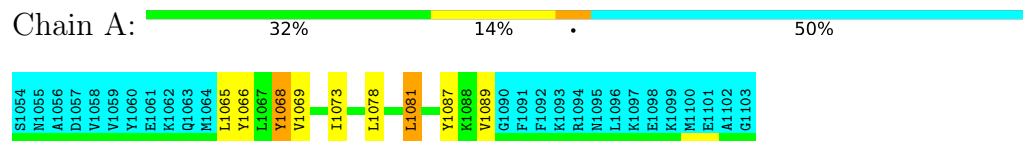
### 4.2.10 Score per residue for model 10

- Molecule 1: Integrin alpha-L



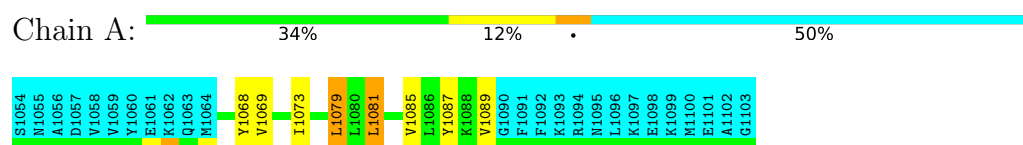
### 4.2.11 Score per residue for model 11

- Molecule 1: Integrin alpha-L



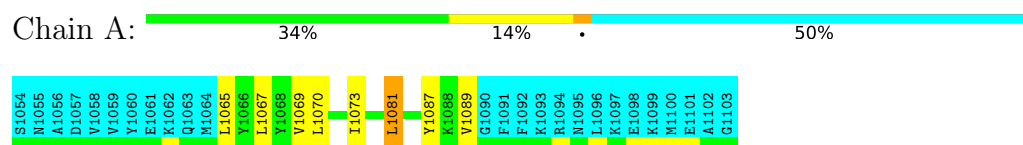
### 4.2.12 Score per residue for model 12

- Molecule 1: Integrin alpha-L



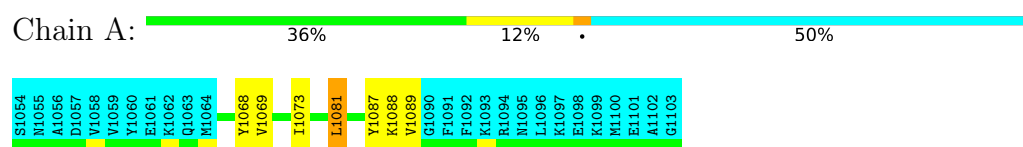
### 4.2.13 Score per residue for model 13

- Molecule 1: Integrin alpha-L



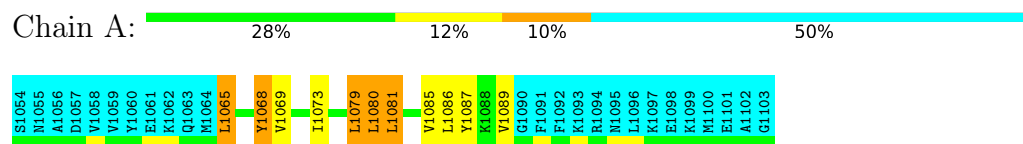
### 4.2.14 Score per residue for model 14

- Molecule 1: Integrin alpha-L



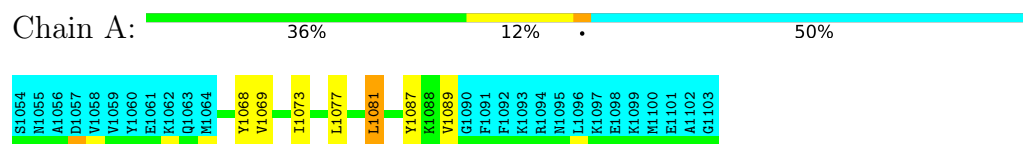
### 4.2.15 Score per residue for model 15

- Molecule 1: Integrin alpha-L



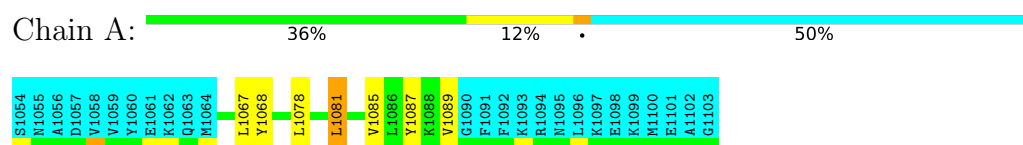
### 4.2.16 Score per residue for model 16

- Molecule 1: Integrin alpha-L



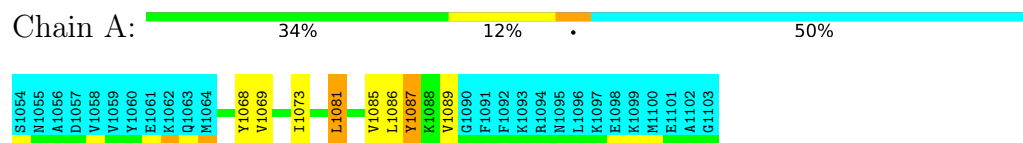
### 4.2.17 Score per residue for model 17

- Molecule 1: Integrin alpha-L



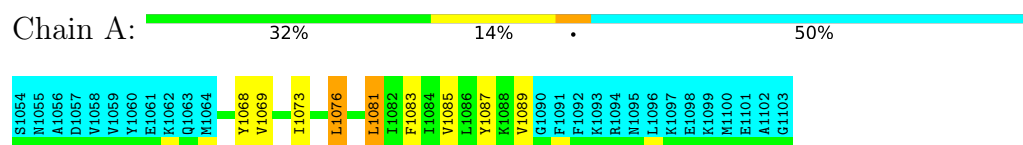
#### 4.2.18 Score per residue for model 18

- Molecule 1: Integrin alpha-L



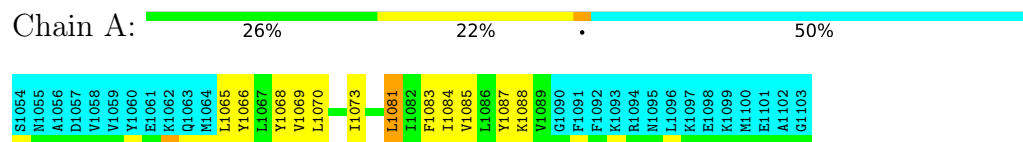
#### 4.2.19 Score per residue for model 19

- Molecule 1: Integrin alpha-L



#### 4.2.20 Score per residue for model 20

- Molecule 1: Integrin alpha-L



## 5 Refinement protocol and experimental data overview

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

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

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

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

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 632            |
| Number of shifts mapped to atoms             | 632            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 86%            |

## 6 Model quality

### 6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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     | 199   | 233      | 233      | 5±2     |
| All | All   | 3980  | 4660     | 4660     | 97      |

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 11.

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

| Atom-1            | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-------------------|-------------------|----------|-------------|--------|-------|
|                   |                   |          |             | Worst  | Total |
| 1:A:1068:TYR:CE2  | 1:A:1069:VAL:HG23 | 0.64     | 2.28        | 11     | 1     |
| 1:A:1078:LEU:HD12 | 1:A:1082:ILE:HD11 | 0.56     | 1.77        | 5      | 1     |
| 1:A:1085:VAL:O    | 1:A:1089:VAL:HG13 | 0.55     | 2.02        | 18     | 11    |
| 1:A:1078:LEU:HD12 | 1:A:1082:ILE:CD1  | 0.54     | 2.33        | 5      | 1     |
| 1:A:1081:LEU:C    | 1:A:1081:LEU:HD12 | 0.53     | 2.29        | 5      | 20    |
| 1:A:1084:ILE:HG22 | 1:A:1088:LYS:CE   | 0.53     | 2.34        | 20     | 1     |
| 1:A:1079:LEU:O    | 1:A:1079:LEU:HD13 | 0.52     | 2.05        | 5      | 6     |
| 1:A:1073:ILE:O    | 1:A:1077:LEU:HD13 | 0.51     | 2.05        | 7      | 1     |
| 1:A:1065:LEU:HD23 | 1:A:1068:TYR:CD2  | 0.51     | 2.40        | 15     | 1     |
| 1:A:1065:LEU:HD12 | 1:A:1066:TYR:N    | 0.50     | 2.21        | 3      | 3     |
| 1:A:1069:VAL:O    | 1:A:1073:ILE:HG23 | 0.49     | 2.06        | 19     | 18    |
| 1:A:1070:LEU:HD12 | 1:A:1073:ILE:HD11 | 0.48     | 1.84        | 20     | 4     |
| 1:A:1080:LEU:O    | 1:A:1080:LEU:HD13 | 0.47     | 2.10        | 9      | 2     |
| 1:A:1076:LEU:C    | 1:A:1076:LEU:HD12 | 0.47     | 2.35        | 19     | 1     |

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| Atom-1            | Atom-2            | Clash(Å) | Distance(Å) | Models |       |
|-------------------|-------------------|----------|-------------|--------|-------|
|                   |                   |          |             | Worst  | Total |
| 1:A:1081:LEU:HD12 | 1:A:1081:LEU:O    | 0.47     | 2.09        | 5      | 1     |
| 1:A:1072:GLY:O    | 1:A:1076:LEU:HD13 | 0.46     | 2.11        | 1      | 1     |
| 1:A:1081:LEU:O    | 1:A:1085:VAL:HG23 | 0.44     | 2.12        | 15     | 8     |
| 1:A:1077:LEU:C    | 1:A:1077:LEU:HD12 | 0.43     | 2.39        | 8      | 1     |
| 1:A:1077:LEU:CD1  | 1:A:1078:LEU:HD12 | 0.43     | 2.44        | 8      | 1     |
| 1:A:1085:VAL:O    | 1:A:1089:VAL:HG22 | 0.42     | 2.15        | 19     | 3     |
| 1:A:1086:LEU:HD12 | 1:A:1087:TYR:N    | 0.42     | 2.29        | 18     | 1     |
| 1:A:1078:LEU:HA   | 1:A:1081:LEU:HD23 | 0.42     | 1.92        | 1      | 6     |
| 1:A:1081:LEU:C    | 1:A:1081:LEU:CD1  | 0.41     | 2.93        | 5      | 1     |
| 1:A:1078:LEU:O    | 1:A:1082:ILE:HD12 | 0.40     | 2.16        | 9      | 3     |

## 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     | 25/50 (50%)    | 25±0 (100±0%) | 0±0 (0±0%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 500/1000 (50%) | 500 (100%)    | 0 (0%)     | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

### 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     | 22/43 (51%)   | 17±1 (79±5%) | 5±1 (21±5%) | 3           | 31 |
| All | All   | 440/860 (51%) | 348 (79%)    | 92 (21%)    | 3           | 31 |

All 13 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     | 1081 | LEU  | 20             |
| 1   | A     | 1087 | TYR  | 20             |
| 1   | A     | 1068 | TYR  | 18             |
| 1   | A     | 1089 | VAL  | 8              |
| 1   | A     | 1079 | LEU  | 7              |
| 1   | A     | 1065 | LEU  | 4              |
| 1   | A     | 1077 | LEU  | 3              |
| 1   | A     | 1080 | LEU  | 3              |
| 1   | A     | 1088 | LYS  | 3              |
| 1   | A     | 1067 | LEU  | 2              |
| 1   | A     | 1083 | PHE  | 2              |
| 1   | A     | 1078 | LEU  | 1              |
| 1   | A     | 1076 | LEU  | 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 86% for the well-defined parts and 85% 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                  | 632 |
| Number of shifts mapped to atoms        | 632 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 1   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action         |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 50       | $2.30 \pm 0.08$                 | Should be checked        |
| $^{13}\text{C}_\beta$  | 45       | $3.49 \pm 0.09$                 | Should be checked        |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data) |
| $^{15}\text{N}$        | 50       | $0.70 \pm 0.34$                 | Should be applied        |

#### 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 86%, i.e. 339 atoms were assigned a chemical shift out of a possible 392. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 103/128 (80%) | 53/53 (100%)   | 25/50 (50%)     | 25/25 (100%)    |
| Sidechain | 209/227 (92%) | 156/156 (100%) | 53/70 (76%)     | 0/1 (0%)        |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 27/37 (73%)   | 17/17 (100%)   | 10/20 (50%)     | 0/0 (—%)        |
| Overall  | 339/392 (86%) | 226/226 (100%) | 88/140 (63%)    | 25/26 (96%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 631 atoms were assigned a chemical shift out of a possible 740. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 204/255 (80%) | 104/105 (99%)  | 50/100 (50%)    | 50/50 (100%)    |
| Sidechain | 382/419 (91%) | 274/278 (99%)  | 104/130 (80%)   | 4/11 (36%)      |
| Aromatic  | 45/66 (68%)   | 29/31 (94%)    | 16/35 (46%)     | 0/0 (—%)        |
| Overall   | 631/740 (85%) | 407/414 (98%)  | 170/265 (64%)   | 54/61 (89%)     |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

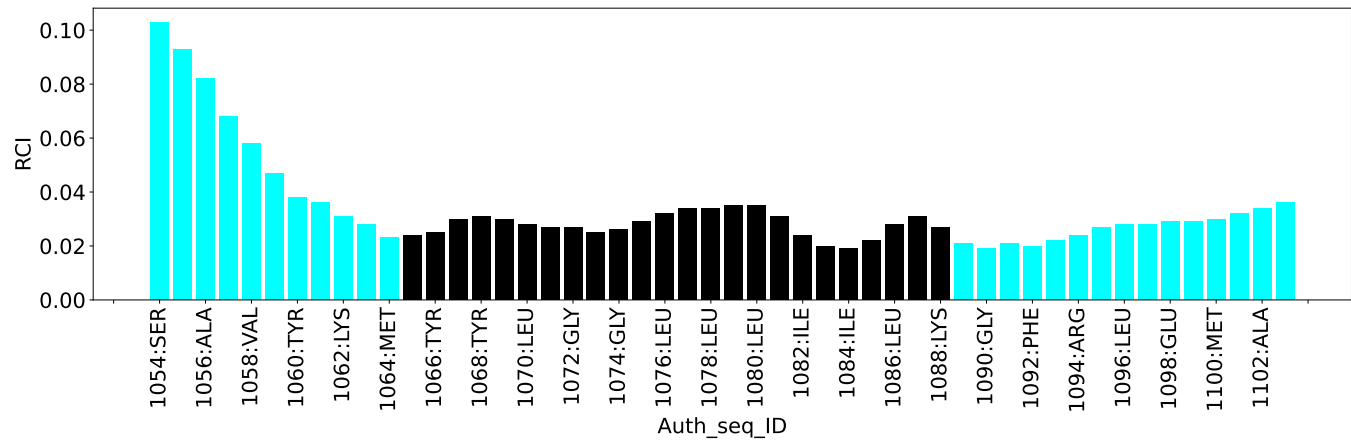
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res  | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|------|------|------|------------|---------------------|---------|
| 1       | A     | 1064 | MET  | CB   | 21.67      | 22.22 – 43.61       | -5.3    |

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

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                                | 564   |
| Intra-residue ( $ i-j =0$ )                              | 230   |
| Sequential ( $ i-j =1$ )                                 | 156   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 155   |
| Long range ( $ i-j \geq 5$ )                             | 23    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 11.3  |
| Number of long range restraints per residue <sup>1</sup> | 0.5   |

<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)  | 9.4                                    | 0.2     |
| 0.2-0.5 (Medium) | 11.1                                   | 0.49    |
| >0.5 (Large)     | 10.6                                   | 2.68    |

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

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

## 9 Distance violation analysis ⓘ

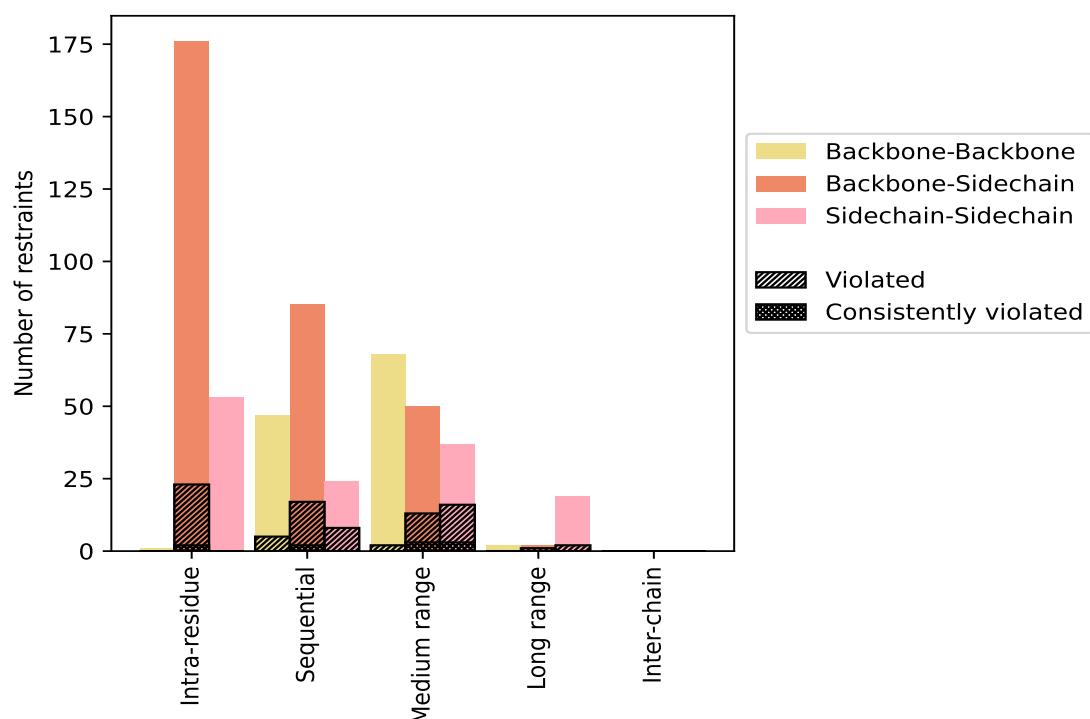
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count               | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                     |                     |
|------------------------------------------------------------|---------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|---------------------|---------------------|
|                                                            |                     |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>      | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">230</a> | <a href="#">40.8</a>  | <a href="#">23</a>    | <a href="#">10.0</a> | <a href="#">4.1</a>  | <a href="#">2</a>                  | <a href="#">0.9</a> | <a href="#">0.4</a> |
| Backbone-Backbone                                          | 1                   | 0.2                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 176                 | 31.2                  | 23                    | 13.1                 | 4.1                  | 2                                  | 1.1                 | 0.4                 |
| Sidechain-Sidechain                                        | 53                  | 9.4                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">156</a> | <a href="#">27.7</a>  | <a href="#">30</a>    | <a href="#">19.2</a> | <a href="#">5.3</a>  | <a href="#">2</a>                  | <a href="#">1.3</a> | <a href="#">0.4</a> |
| Backbone-Backbone                                          | 47                  | 8.3                   | 5                     | 10.6                 | 0.9                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 85                  | 15.1                  | 17                    | 20.0                 | 3.0                  | 2                                  | 2.4                 | 0.4                 |
| Sidechain-Sidechain                                        | 24                  | 4.3                   | 8                     | 33.3                 | 1.4                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">155</a> | <a href="#">27.5</a>  | <a href="#">31</a>    | <a href="#">20.0</a> | <a href="#">5.5</a>  | <a href="#">6</a>                  | <a href="#">3.9</a> | <a href="#">1.1</a> |
| Backbone-Backbone                                          | 68                  | 12.1                  | 2                     | 2.9                  | 0.4                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 50                  | 8.9                   | 13                    | 26.0                 | 2.3                  | 3                                  | 6.0                 | 0.5                 |
| Sidechain-Sidechain                                        | 37                  | 6.6                   | 16                    | 43.2                 | 2.8                  | 3                                  | 8.1                 | 0.5                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">23</a>  | <a href="#">4.1</a>   | <a href="#">3</a>     | <a href="#">13.0</a> | <a href="#">0.5</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 2                   | 0.4                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 2                   | 0.4                   | 1                     | 50.0                 | 0.2                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 19                  | 3.4                   | 2                     | 10.5                 | 0.4                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">564</a> | <a href="#">100.0</a> | <a href="#">87</a>    | <a href="#">15.4</a> | <a href="#">15.4</a> | <a href="#">10</a>                 | <a href="#">1.8</a> | <a href="#">1.8</a> |
| Backbone-Backbone                                          | 118                 | 20.9                  | 7                     | 5.9                  | 1.2                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 313                 | 55.5                  | 54                    | 17.3                 | 9.6                  | 7                                  | 2.2                 | 1.2                 |
| Sidechain-Sidechain                                        | 133                 | 23.6                  | 26                    | 19.5                 | 4.6                  | 3                                  | 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        | 8                    | 8               | 11              | 1               | 0               | 28    | 0.46     | 2.09    | 0.5                 | 0.27       |
| 2        | 8                    | 13              | 17              | 2               | 0               | 40    | 0.76     | 2.68    | 0.74                | 0.4        |
| 3        | 6                    | 8               | 13              | 1               | 0               | 28    | 0.51     | 2.28    | 0.53                | 0.3        |
| 4        | 6                    | 7               | 13              | 0               | 0               | 26    | 0.53     | 2.21    | 0.63                | 0.26       |
| 5        | 8                    | 9               | 14              | 1               | 0               | 32    | 0.49     | 2.11    | 0.5                 | 0.32       |
| 6        | 4                    | 8               | 13              | 1               | 0               | 26    | 0.52     | 2.09    | 0.52                | 0.32       |
| 7        | 6                    | 9               | 13              | 1               | 0               | 29    | 0.45     | 2.12    | 0.5                 | 0.27       |
| 8        | 5                    | 12              | 14              | 1               | 0               | 32    | 0.55     | 2.34    | 0.63                | 0.29       |
| 9        | 9                    | 10              | 16              | 1               | 0               | 36    | 0.49     | 2.07    | 0.47                | 0.33       |
| 10       | 8                    | 8               | 13              | 0               | 0               | 29    | 0.47     | 2.13    | 0.51                | 0.24       |

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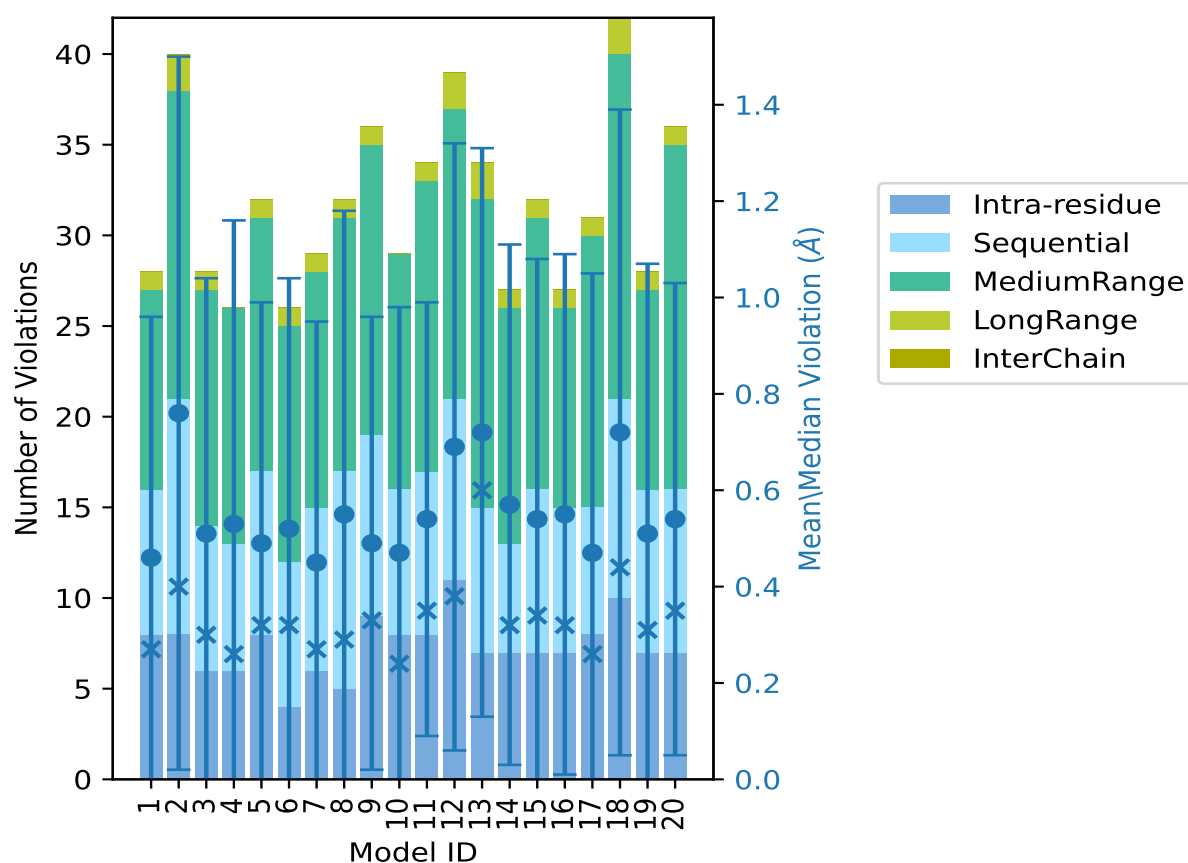
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 8                    | 9               | 16              | 1               | 0               | 34    | 0.54     | 2.14    | 0.45                | 0.35       |
| 12       | 11                   | 10              | 16              | 2               | 0               | 39    | 0.69     | 2.28    | 0.63                | 0.38       |
| 13       | 7                    | 8               | 17              | 2               | 0               | 34    | 0.72     | 2.45    | 0.59                | 0.6        |
| 14       | 7                    | 6               | 13              | 1               | 0               | 27    | 0.57     | 1.82    | 0.54                | 0.32       |
| 15       | 7                    | 9               | 15              | 1               | 0               | 32    | 0.54     | 2.1     | 0.54                | 0.34       |
| 16       | 7                    | 8               | 11              | 1               | 0               | 27    | 0.55     | 2.12    | 0.54                | 0.32       |
| 17       | 8                    | 7               | 15              | 1               | 0               | 31    | 0.47     | 2.38    | 0.58                | 0.26       |
| 18       | 10                   | 11              | 19              | 2               | 0               | 42    | 0.72     | 2.68    | 0.67                | 0.44       |
| 19       | 7                    | 9               | 11              | 1               | 0               | 28    | 0.51     | 2.12    | 0.56                | 0.31       |
| 20       | 7                    | 9               | 19              | 1               | 0               | 36    | 0.54     | 2.07    | 0.49                | 0.35       |

<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

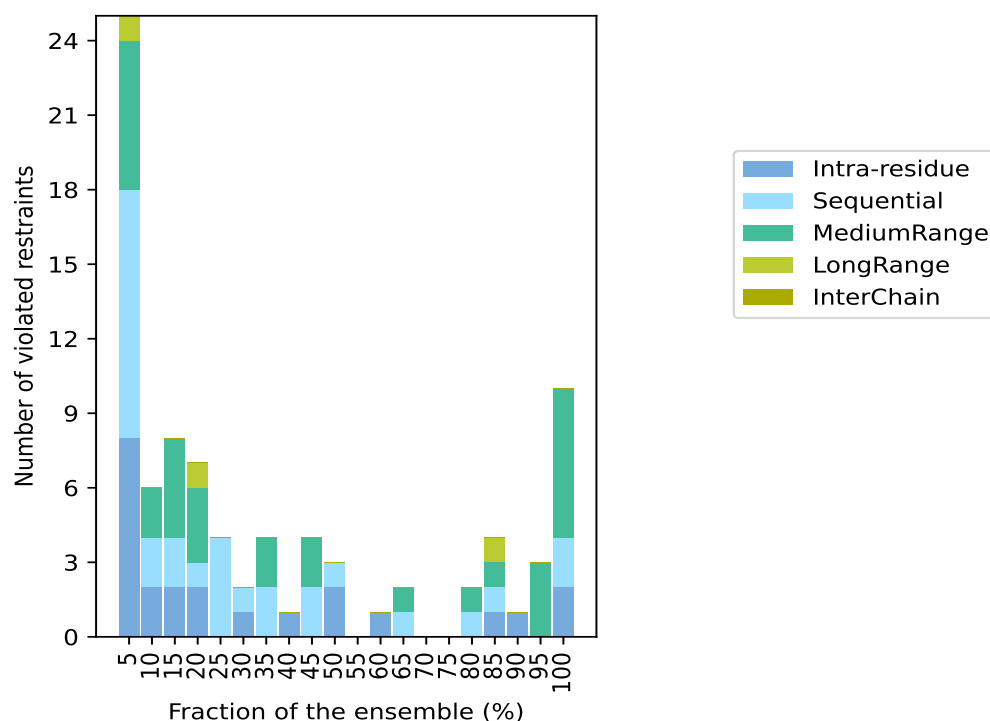
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 477(IR:207, SQ:126, MR:124, LR:20, IC:0) restraints are not 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>       | %     |
| 8                             | 10              | 6               | 1               | 0               | 25    | 1                        | 5.0   |
| 2                             | 2               | 2               | 0               | 0               | 6     | 2                        | 10.0  |
| 2                             | 2               | 4               | 0               | 0               | 8     | 3                        | 15.0  |
| 2                             | 1               | 3               | 1               | 0               | 7     | 4                        | 20.0  |
| 0                             | 4               | 0               | 0               | 0               | 4     | 5                        | 25.0  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 6                        | 30.0  |
| 0                             | 2               | 2               | 0               | 0               | 4     | 7                        | 35.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 8                        | 40.0  |
| 0                             | 2               | 2               | 0               | 0               | 4     | 9                        | 45.0  |
| 2                             | 1               | 0               | 0               | 0               | 3     | 10                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 55.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 12                       | 60.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 13                       | 65.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 15                       | 75.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 16                       | 80.0  |
| 1                             | 1               | 1               | 1               | 0               | 4     | 17                       | 85.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 18                       | 90.0  |
| 0                             | 0               | 3               | 0               | 0               | 3     | 19                       | 95.0  |
| 2                             | 2               | 6               | 0               | 0               | 10    | 20                       | 100.0 |

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

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

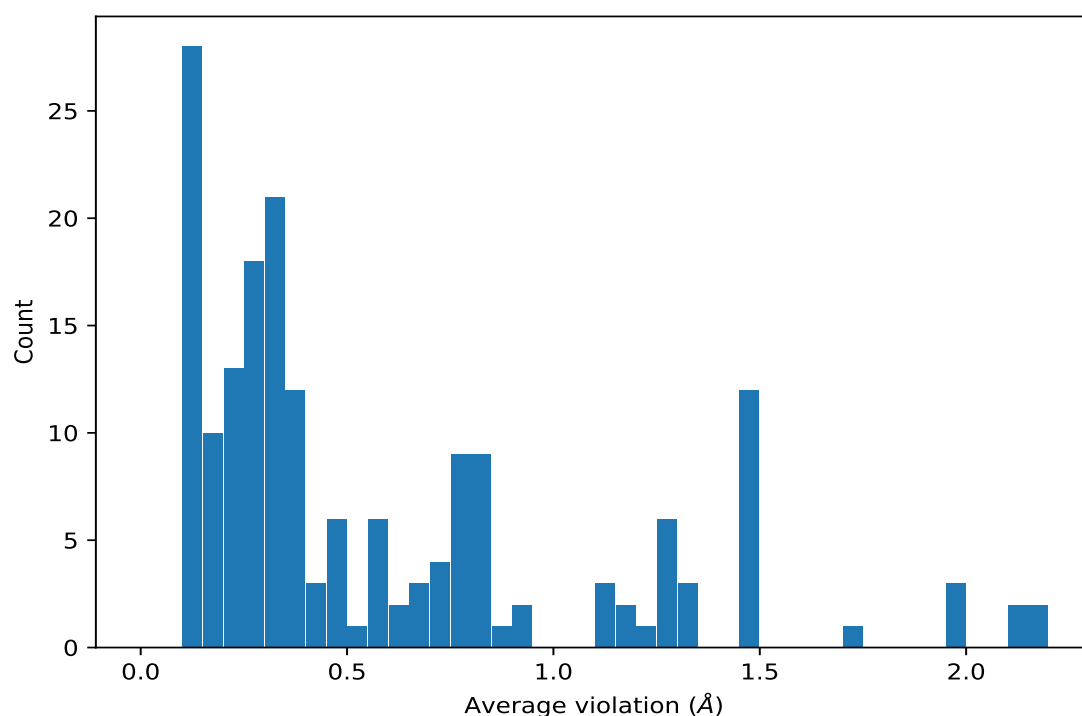
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG   | 20                  | 2.1      | 0.08                | 2.11       |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG   | 20                  | 2.1      | 0.08                | 2.11       |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 20                  | 1.48     | 0.52                | 1.43       |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 20                  | 1.25     | 0.05                | 1.24       |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 20                  | 1.25     | 0.05                | 1.24       |

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| Key     | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 20                  | 1.25     | 0.05                | 1.24       |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 20                  | 0.63     | 0.18                | 0.76       |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 20                  | 0.63     | 0.18                | 0.76       |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 20                  | 0.54     | 0.01                | 0.54       |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 20                  | 0.35     | 0.02                | 0.35       |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 20                  | 0.35     | 0.02                | 0.35       |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 20                  | 0.35     | 0.02                | 0.35       |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 20                  | 0.35     | 0.02                | 0.35       |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 20                  | 0.32     | 0.08                | 0.31       |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 20                  | 0.32     | 0.08                | 0.31       |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 20                  | 0.3      | 0.01                | 0.3        |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 20                  | 0.3      | 0.01                | 0.3        |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 20                  | 0.3      | 0.02                | 0.31       |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 20                  | 0.3      | 0.02                | 0.31       |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 20                  | 0.16     | 0.03                | 0.15       |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 19                  | 0.35     | 0.08                | 0.35       |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 19                  | 0.18     | 0.06                | 0.19       |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 19                  | 0.14     | 0.01                | 0.14       |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 19                  | 0.14     | 0.01                | 0.14       |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 19                  | 0.14     | 0.01                | 0.14       |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 19                  | 0.14     | 0.01                | 0.14       |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 18                  | 0.36     | 0.21                | 0.28       |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 18                  | 0.36     | 0.21                | 0.28       |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H    | 17                  | 1.72     | 0.1                 | 1.75       |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 17                  | 0.27     | 0.11                | 0.24       |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 17                  | 0.27     | 0.11                | 0.24       |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 17                  | 0.27     | 0.11                | 0.24       |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 17                  | 0.27     | 0.11                | 0.24       |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 17                  | 0.27     | 0.11                | 0.24       |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 17                  | 0.27     | 0.11                | 0.24       |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 17                  | 0.26     | 0.1                 | 0.25       |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 17                  | 0.26     | 0.1                 | 0.25       |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 17                  | 0.26     | 0.1                 | 0.25       |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 17                  | 0.17     | 0.01                | 0.17       |

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| Key     | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 17                  | 0.17     | 0.01                | 0.17       |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 16                  | 0.4      | 0.12                | 0.43       |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 16                  | 0.4      | 0.12                | 0.43       |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG21 | 16                  | 0.14     | 0.01                | 0.15       |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG22 | 16                  | 0.14     | 0.01                | 0.15       |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG23 | 16                  | 0.14     | 0.01                | 0.15       |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 16                  | 0.14     | 0.01                | 0.15       |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 16                  | 0.14     | 0.01                | 0.15       |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 16                  | 0.14     | 0.01                | 0.15       |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 13                  | 1.17     | 0.66                | 1.52       |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 13                  | 1.17     | 0.66                | 1.52       |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 13                  | 0.76     | 0.48                | 0.74       |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 13                  | 0.76     | 0.48                | 0.74       |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 13                  | 0.76     | 0.48                | 0.74       |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 13                  | 0.76     | 0.48                | 0.74       |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 13                  | 0.76     | 0.48                | 0.74       |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 13                  | 0.76     | 0.48                | 0.74       |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 12                  | 0.11     | 0.02                | 0.11       |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 12                  | 0.11     | 0.02                | 0.11       |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 12                  | 0.11     | 0.02                | 0.11       |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 10                  | 0.46     | 0.14                | 0.5        |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 10                  | 0.2      | 0.07                | 0.19       |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 10                  | 0.2      | 0.07                | 0.19       |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 10                  | 0.2      | 0.07                | 0.19       |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 10                  | 0.16     | 0.03                | 0.16       |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H    | 9                   | 1.1      | 0.52                | 0.71       |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H    | 9                   | 1.1      | 0.52                | 0.71       |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H    | 9                   | 1.1      | 0.52                | 0.71       |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG11 | 9                   | 0.72     | 0.18                | 0.77       |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG12 | 9                   | 0.72     | 0.18                | 0.77       |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG13 | 9                   | 0.72     | 0.18                | 0.77       |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 9                   | 0.21     | 0.04                | 0.21       |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 9                   | 0.19     | 0.05                | 0.21       |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 9                   | 0.19     | 0.05                | 0.21       |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 8                   | 0.3      | 0.02                | 0.3        |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 8                   | 0.3      | 0.02                | 0.3        |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 8                   | 0.3      | 0.02                | 0.3        |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD11 | 7                   | 1.31     | 0.03                | 1.32       |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD12 | 7                   | 1.31     | 0.03                | 1.32       |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD13 | 7                   | 1.31     | 0.03                | 1.32       |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG2  | 7                   | 0.9      | 0.78                | 0.94       |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG3  | 7                   | 0.9      | 0.78                | 0.94       |

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| Key     | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB2  | 7                   | 0.49     | 0.23                | 0.65       |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB3  | 7                   | 0.49     | 0.23                | 0.65       |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB2  | 7                   | 0.49     | 0.23                | 0.65       |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB3  | 7                   | 0.49     | 0.23                | 0.65       |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB2  | 7                   | 0.13     | 0.01                | 0.14       |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB3  | 7                   | 0.13     | 0.01                | 0.14       |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD21 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD22 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD23 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD21 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD22 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD23 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD21 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD22 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD23 | 6                   | 0.36     | 0.31                | 0.24       |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE1  | 6                   | 0.15     | 0.05                | 0.12       |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE2  | 6                   | 0.15     | 0.05                | 0.12       |
| (1,519) | 1:1096:A:LEU:HA   | 1:1097:A:LYS:H    | 5                   | 0.45     | 0.01                | 0.46       |
| (1,46)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 5                   | 0.41     | 0.1                 | 0.44       |
| (1,41)  | 1:1062:A:LYS:H    | 1:1063:A:GLN:H    | 5                   | 0.37     | 0.09                | 0.43       |
| (1,67)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 5                   | 0.22     | 0.04                | 0.24       |
| (1,67)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 5                   | 0.22     | 0.04                | 0.24       |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD2  | 4                   | 2.15     | 0.54                | 2.18       |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD3  | 4                   | 2.15     | 0.54                | 2.18       |
| (1,345) | 1:1084:A:ILE:HD11 | 1:1087:A:TYR:HD1  | 4                   | 1.96     | 0.75                | 2.37       |
| (1,345) | 1:1084:A:ILE:HD12 | 1:1087:A:TYR:HD1  | 4                   | 1.96     | 0.75                | 2.37       |
| (1,345) | 1:1084:A:ILE:HD13 | 1:1087:A:TYR:HD1  | 4                   | 1.96     | 0.75                | 2.37       |
| (1,348) | 1:1084:A:ILE:HG21 | 1:1087:A:TYR:HD1  | 4                   | 1.29     | 0.1                 | 1.31       |
| (1,348) | 1:1084:A:ILE:HG22 | 1:1087:A:TYR:HD1  | 4                   | 1.29     | 0.1                 | 1.31       |
| (1,348) | 1:1084:A:ILE:HG23 | 1:1087:A:TYR:HD1  | 4                   | 1.29     | 0.1                 | 1.31       |
| (1,415) | 1:1087:A:TYR:HD1  | 1:1089:A:VAL:H    | 4                   | 1.24     | 0.09                | 1.24       |
| (1,414) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:H    | 4                   | 0.87     | 0.04                | 0.87       |
| (1,413) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HD1  | 4                   | 0.73     | 0.01                | 0.72       |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG21 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG22 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG23 | 4                   | 0.1      | 0.0                 | 0.1        |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG11 | 3                   | 0.8      | 0.88                | 0.21       |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG12 | 3                   | 0.8      | 0.88                | 0.21       |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG13 | 3                   | 0.8      | 0.88                | 0.21       |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG11 | 3                   | 0.8      | 0.88                | 0.21       |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG12 | 3                   | 0.8      | 0.88                | 0.21       |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG13 | 3                   | 0.8      | 0.88                | 0.21       |

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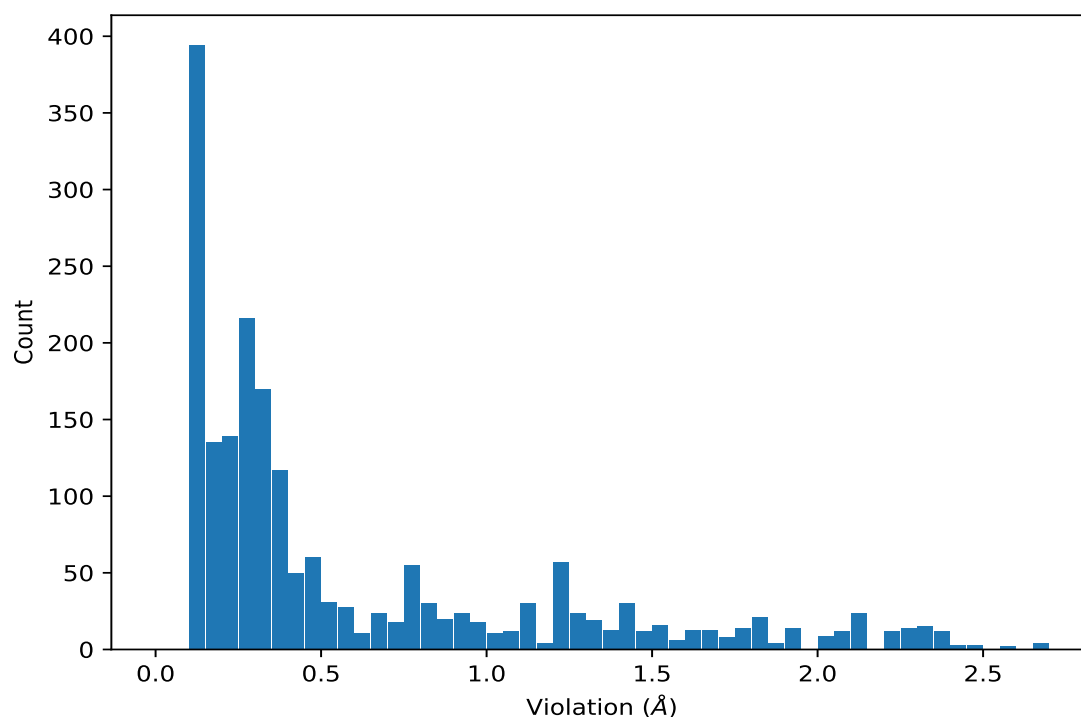
| Key     | Atom-1            | Atom-2            | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-------------------|-------------------|---------------------|----------|---------------------|------------|
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG11 | 3                   | 0.8      | 0.88                | 0.21       |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG12 | 3                   | 0.8      | 0.88                | 0.21       |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG13 | 3                   | 0.8      | 0.88                | 0.21       |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD11 | 3                   | 0.79     | 0.45                | 0.91       |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD12 | 3                   | 0.79     | 0.45                | 0.91       |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD13 | 3                   | 0.79     | 0.45                | 0.91       |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD11 | 3                   | 0.68     | 0.32                | 0.9        |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD12 | 3                   | 0.68     | 0.32                | 0.9        |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD13 | 3                   | 0.68     | 0.32                | 0.9        |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD11 | 3                   | 0.59     | 0.23                | 0.58       |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD12 | 3                   | 0.59     | 0.23                | 0.58       |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD13 | 3                   | 0.59     | 0.23                | 0.58       |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD11 | 3                   | 0.59     | 0.23                | 0.58       |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD12 | 3                   | 0.59     | 0.23                | 0.58       |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD13 | 3                   | 0.59     | 0.23                | 0.58       |
| (1,21)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 3                   | 0.35     | 0.11                | 0.38       |
| (1,21)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 3                   | 0.35     | 0.11                | 0.38       |
| (1,21)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 3                   | 0.35     | 0.11                | 0.38       |
| (1,21)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 3                   | 0.35     | 0.11                | 0.38       |
| (1,21)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 3                   | 0.35     | 0.11                | 0.38       |
| (1,21)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 3                   | 0.35     | 0.11                | 0.38       |
| (1,90)  | 1:1065:A:LEU:HA   | 1:1065:A:LEU:HG   | 3                   | 0.2      | 0.0                 | 0.2        |
| (1,366) | 1:1085:A:VAL:H    | 1:1086:A:LEU:HG   | 3                   | 0.17     | 0.04                | 0.17       |
| (1,409) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HE1  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,409) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HE2  | 3                   | 0.12     | 0.0                 | 0.12       |
| (1,477) | 1:1092:A:PHE:H    | 1:1093:A:LYS:HB2  | 2                   | 0.25     | 0.11                | 0.25       |
| (1,477) | 1:1092:A:PHE:H    | 1:1093:A:LYS:HB3  | 2                   | 0.25     | 0.11                | 0.25       |
| (1,18)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,18)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,18)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,18)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,18)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,18)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:H    | 2                   | 0.24     | 0.0                 | 0.24       |
| (1,14)  | 1:1058:A:VAL:H    | 1:1058:A:VAL:HB   | 2                   | 0.17     | 0.02                | 0.17       |
| (1,531) | 1:1097:A:LYS:HB2  | 1:1098:A:GLU:H    | 2                   | 0.16     | 0.04                | 0.16       |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG11 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG12 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG13 | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD21 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD23 | 2                   | 0.12     | 0.02                | 0.12       |

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

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

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

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



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

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

| Key     | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|---------|-------------------|------------------|----------|---------------|
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD2 | 2        | 2.68          |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD3 | 2        | 2.68          |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD2 | 18       | 2.68          |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD3 | 18       | 2.68          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG2 | 2        | 2.57          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG3 | 2        | 2.57          |
| (1,345) | 1:1084:A:ILE:HD11 | 1:1087:A:TYR:HD1 | 13       | 2.45          |
| (1,345) | 1:1084:A:ILE:HD12 | 1:1087:A:TYR:HD1 | 13       | 2.45          |
| (1,345) | 1:1084:A:ILE:HD13 | 1:1087:A:TYR:HD1 | 13       | 2.45          |
| (1,345) | 1:1084:A:ILE:HD11 | 1:1087:A:TYR:HD1 | 2        | 2.41          |

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| Key     | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|---------|-------------------|------------------|----------|---------------|
| (1,345) | 1:1084:A:ILE:HD12 | 1:1087:A:TYR:HD1 | 2        | 2.41          |
| (1,345) | 1:1084:A:ILE:HD13 | 1:1087:A:TYR:HD1 | 2        | 2.41          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2 | 17       | 2.38          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1 | 8        | 2.34          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2 | 8        | 2.34          |
| (1,345) | 1:1084:A:ILE:HD11 | 1:1087:A:TYR:HD1 | 18       | 2.32          |
| (1,345) | 1:1084:A:ILE:HD12 | 1:1087:A:TYR:HD1 | 18       | 2.32          |
| (1,345) | 1:1084:A:ILE:HD13 | 1:1087:A:TYR:HD1 | 18       | 2.32          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 3        | 2.28          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 3        | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1 | 12       | 2.28          |

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| Key     | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|---------|-------------------|------------------|----------|---------------|
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2 | 12       | 2.28          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1 | 4        | 2.21          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2 | 4        | 2.21          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 11       | 2.14          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 11       | 2.14          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 2        | 2.13          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 2        | 2.13          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 10       | 2.13          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 10       | 2.13          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 18       | 2.13          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 18       | 2.13          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 7        | 2.12          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 7        | 2.12          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 8        | 2.12          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 8        | 2.12          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 16       | 2.12          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 16       | 2.12          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 19       | 2.12          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 19       | 2.12          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 5        | 2.11          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 5        | 2.11          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 12       | 2.11          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 12       | 2.11          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 4        | 2.1           |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 4        | 2.1           |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 15       | 2.1           |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 15       | 2.1           |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 1        | 2.09          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 1        | 2.09          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 6        | 2.09          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG  | 6        | 2.09          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG  | 9        | 2.07          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG   | 9        | 2.07          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG   | 20       | 2.07          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG   | 20       | 2.07          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG   | 13       | 2.06          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG   | 13       | 2.06          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG   | 17       | 2.06          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG   | 17       | 2.06          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG11 | 18       | 2.04          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG12 | 18       | 2.04          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG13 | 18       | 2.04          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG11 | 18       | 2.04          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG12 | 18       | 2.04          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG13 | 18       | 2.04          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG11 | 18       | 2.04          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG12 | 18       | 2.04          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG13 | 18       | 2.04          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 19       | 1.94          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 19       | 1.94          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 12       | 1.91          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 12       | 1.91          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 8        | 1.9           |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 8        | 1.9           |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 15       | 1.88          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 15       | 1.88          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H    | 4        | 1.83          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H    | 8        | 1.83          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H    | 17       | 1.83          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H    | 1        | 1.82          |
| (1,111) | 1:1066:A:TYR:HD1  | 1:1070:A:LEU:HG   | 14       | 1.82          |
| (1,111) | 1:1066:A:TYR:HD2  | 1:1070:A:LEU:HG   | 14       | 1.82          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H    | 19       | 1.81          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H    | 12       | 1.8           |

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| Key     | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|---------|-------------------|------------------|----------|---------------|
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 15       | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2 | 2        | 1.8           |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1 | 14       | 1.78          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2 | 14       | 1.78          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 16       | 1.76          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 3        | 1.75          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2 | 2        | 1.74          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3 | 2        | 1.74          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2 | 7        | 1.74          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3 | 7        | 1.74          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 5        | 1.71          |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H   | 12       | 1.71          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H   | 12       | 1.71          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H   | 12       | 1.71          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 14       | 1.7           |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD2 | 13       | 1.69          |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD3 | 13       | 1.69          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 10       | 1.67          |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H   | 2        | 1.67          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H   | 2        | 1.67          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H   | 2        | 1.67          |

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| Key     | Atom-1            | Atom-2           | Model ID | Violation (Å) |
|---------|-------------------|------------------|----------|---------------|
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H   | 14       | 1.66          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H   | 14       | 1.66          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H   | 14       | 1.66          |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H   | 16       | 1.66          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H   | 16       | 1.66          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H   | 16       | 1.66          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1 | 20       | 1.64          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2 | 20       | 1.64          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 18       | 1.63          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 9        | 1.58          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2 | 5        | 1.58          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3 | 5        | 1.58          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 13       | 1.57          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 2        | 1.56          |
| (1,534) | 1:1097:A:LYS:H    | 1:1098:A:GLU:H   | 11       | 1.55          |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD2 | 12       | 1.54          |
| (1,416) | 1:1087:A:TYR:HD2  | 1:1093:A:LYS:HD3 | 12       | 1.54          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1 | 6        | 1.53          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2 | 6        | 1.53          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2 | 6        | 1.52          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3 | 6        | 1.52          |
| (1,393) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:H   | 18       | 1.48          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,393) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:H    | 18       | 1.48          |
| (1,393) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:H    | 18       | 1.48          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 20       | 1.46          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 20       | 1.46          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 20       | 1.46          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 20       | 1.46          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 20       | 1.46          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 20       | 1.46          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 20       | 1.46          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 20       | 1.46          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 20       | 1.46          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 9        | 1.44          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 9        | 1.44          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 9        | 1.44          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 9        | 1.44          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 9        | 1.44          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 9        | 1.44          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 10       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 13       | 1.43          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 13       | 1.43          |
| (1,348) | 1:1084:A:ILE:HG21 | 1:1087:A:TYR:HD1  | 12       | 1.4           |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,348) | 1:1084:A:ILE:HG22 | 1:1087:A:TYR:HD1  | 12       | 1.4           |
| (1,348) | 1:1084:A:ILE:HG23 | 1:1087:A:TYR:HD1  | 12       | 1.4           |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 18       | 1.38          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 18       | 1.38          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 18       | 1.38          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 18       | 1.38          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 18       | 1.38          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 18       | 1.38          |
| (1,415) | 1:1087:A:TYR:HD1  | 1:1089:A:VAL:H    | 13       | 1.35          |
| (1,348) | 1:1084:A:ILE:HG21 | 1:1087:A:TYR:HD1  | 13       | 1.35          |
| (1,348) | 1:1084:A:ILE:HG22 | 1:1087:A:TYR:HD1  | 13       | 1.35          |
| (1,348) | 1:1084:A:ILE:HG23 | 1:1087:A:TYR:HD1  | 13       | 1.35          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD11 | 4        | 1.33          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD12 | 4        | 1.33          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD13 | 4        | 1.33          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD11 | 9        | 1.33          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD12 | 9        | 1.33          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD13 | 9        | 1.33          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD11 | 12       | 1.32          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD12 | 12       | 1.32          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD13 | 12       | 1.32          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD11 | 15       | 1.32          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD12 | 15       | 1.32          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD13 | 15       | 1.32          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD11 | 6        | 1.31          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD12 | 6        | 1.31          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD13 | 6        | 1.31          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD11 | 8        | 1.31          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD12 | 8        | 1.31          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD13 | 8        | 1.31          |
| (1,415) | 1:1087:A:TYR:HD1  | 1:1089:A:VAL:H    | 18       | 1.3           |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD11 | 3        | 1.27          |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD12 | 3        | 1.27          |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD13 | 3        | 1.27          |
| (1,348) | 1:1084:A:ILE:HG21 | 1:1087:A:TYR:HD1  | 2        | 1.26          |
| (1,348) | 1:1084:A:ILE:HG22 | 1:1087:A:TYR:HD1  | 2        | 1.26          |
| (1,348) | 1:1084:A:ILE:HG23 | 1:1087:A:TYR:HD1  | 2        | 1.26          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 2        | 1.26          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 2        | 1.26          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 2        | 1.26          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 7        | 1.26          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 7        | 1.26          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 7        | 1.26          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 3        | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 3        | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 3        | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 4        | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 4        | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 4        | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 12       | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 12       | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 12       | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 13       | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 13       | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 13       | 1.25          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 1        | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 1        | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 1        | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 6        | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 6        | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 6        | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 11       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 11       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 11       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 14       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 14       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 14       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 15       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 15       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 15       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 16       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 16       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 16       | 1.24          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD11 | 20       | 1.24          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD12 | 20       | 1.24          |
| (1,279) | 1:1081:A:LEU:HA   | 1:1084:A:ILE:HD13 | 20       | 1.24          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 11       | 1.24          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 11       | 1.24          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 11       | 1.24          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 11       | 1.24          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 11       | 1.24          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 11       | 1.24          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 9        | 1.23          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 9        | 1.23          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 9        | 1.23          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 17       | 1.23          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 17       | 1.23          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 17       | 1.23          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 19       | 1.22          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 19       | 1.22          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 19       | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 7        | 1.22          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 7        | 1.22          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 5        | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 5        | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 5        | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 8        | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 8        | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 8        | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 18       | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 18       | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 18       | 1.21          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG21 | 10       | 1.19          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG22 | 10       | 1.19          |
| (1,315) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG23 | 10       | 1.19          |
| (1,415) | 1:1087:A:TYR:HD1  | 1:1089:A:VAL:H    | 12       | 1.18          |
| (1,348) | 1:1084:A:ILE:HG21 | 1:1087:A:TYR:HD1  | 18       | 1.15          |
| (1,348) | 1:1084:A:ILE:HG22 | 1:1087:A:TYR:HD1  | 18       | 1.15          |
| (1,348) | 1:1084:A:ILE:HG23 | 1:1087:A:TYR:HD1  | 18       | 1.15          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG2  | 18       | 1.14          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG3  | 18       | 1.14          |
| (1,415) | 1:1087:A:TYR:HD1  | 1:1089:A:VAL:H    | 2        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 1        | 1.14          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 1        | 1.14          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 5        | 1.11          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 11       | 1.06          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 11       | 1.06          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD21 | 18       | 1.04          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD22 | 18       | 1.04          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD23 | 18       | 1.04          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD21 | 18       | 1.04          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD22 | 18       | 1.04          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD23 | 18       | 1.04          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD21 | 18       | 1.04          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD22 | 18       | 1.04          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD23 | 18       | 1.04          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG2  | 12       | 1.03          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG3  | 12       | 1.03          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 3        | 0.99          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 3        | 0.99          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 15       | 0.98          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 15       | 0.98          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 15       | 0.98          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 15       | 0.98          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 15       | 0.98          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 15       | 0.98          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG2  | 13       | 0.94          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG3  | 13       | 0.94          |
| (1,414) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:H    | 18       | 0.93          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 16       | 0.92          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 16       | 0.92          |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD11 | 11       | 0.91          |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD12 | 11       | 0.91          |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD13 | 11       | 0.91          |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD11 | 20       | 0.91          |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD12 | 20       | 0.91          |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD13 | 20       | 0.91          |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD11 | 20       | 0.9           |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD12 | 20       | 0.9           |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD13 | 20       | 0.9           |
| (1,414) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:H    | 13       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 18       | 0.88          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 18       | 0.88          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD11 | 20       | 0.87          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD12 | 20       | 0.87          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD13 | 20       | 0.87          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD11 | 20       | 0.87          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD12 | 20       | 0.87          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD13 | 20       | 0.87          |
| (1,414) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:H    | 12       | 0.86          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 15       | 0.85          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 15       | 0.85          |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG11 | 20       | 0.84          |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG12 | 20       | 0.84          |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG13 | 20       | 0.84          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 16       | 0.83          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 16       | 0.83          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 16       | 0.83          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 16       | 0.83          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 16       | 0.83          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 16       | 0.83          |

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| Key     | Atom-1           | Atom-2            | Model ID | Violation (Å) |
|---------|------------------|-------------------|----------|---------------|
| (1,414) | 1:1087:A:TYR:HD1 | 1:1088:A:LYS:H    | 2        | 0.81          |
| (1,535) | 1:1097:A:LYS:H   | 1:1097:A:LYS:HD2  | 13       | 0.8           |
| (1,535) | 1:1097:A:LYS:H   | 1:1097:A:LYS:HD3  | 13       | 0.8           |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG11 | 9        | 0.8           |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG12 | 9        | 0.8           |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG13 | 9        | 0.8           |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG11 | 12       | 0.8           |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG12 | 12       | 0.8           |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG13 | 12       | 0.8           |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG11 | 2        | 0.78          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG12 | 2        | 0.78          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG13 | 2        | 0.78          |
| (1,249) | 1:1079:A:LEU:HG  | 1:1083:A:PHE:HB2  | 18       | 0.78          |
| (1,249) | 1:1079:A:LEU:HG  | 1:1083:A:PHE:HB3  | 18       | 0.78          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG11 | 11       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG12 | 11       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG13 | 11       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG11 | 13       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG12 | 13       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG13 | 13       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG11 | 16       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG12 | 16       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG13 | 16       | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG12 | 1        | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG13 | 1        | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG12 | 2        | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG13 | 2        | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG12 | 3        | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG13 | 3        | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG12 | 7        | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG13 | 7        | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG12 | 13       | 0.77          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG13 | 13       | 0.77          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG11 | 14       | 0.76          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG12 | 14       | 0.76          |
| (1,428) | 1:1088:A:LYS:H   | 1:1089:A:VAL:HG13 | 14       | 0.76          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG12 | 5        | 0.76          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG13 | 5        | 0.76          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG12 | 11       | 0.76          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG13 | 11       | 0.76          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG12 | 16       | 0.76          |
| (1,304) | 1:1082:A:ILE:H   | 1:1084:A:ILE:HG13 | 16       | 0.76          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 17       | 0.76          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 17       | 0.76          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 19       | 0.76          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 19       | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD1  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:HD2  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD1  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:HD2  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD1  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:HD2  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 9        | 0.76          |
| (1,19)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 9        | 0.76          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 20       | 0.75          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 20       | 0.75          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 10       | 0.75          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 10       | 0.75          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 14       | 0.75          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 14       | 0.75          |
| (1,413) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HD1  | 18       | 0.74          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 18       | 0.74          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 18       | 0.74          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 19       | 0.74          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 19       | 0.74          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 19       | 0.74          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 19       | 0.74          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 19       | 0.74          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 19       | 0.74          |
| (1,413) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HD1  | 13       | 0.73          |
| (1,436) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG21 | 10       | 0.72          |
| (1,436) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG22 | 10       | 0.72          |
| (1,436) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG23 | 10       | 0.72          |
| (1,413) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HD1  | 2        | 0.72          |
| (1,413) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HD1  | 12       | 0.72          |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H    | 10       | 0.71          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H    | 10       | 0.71          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H    | 10       | 0.71          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB2  | 13       | 0.68          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB3  | 13       | 0.68          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB2  | 13       | 0.68          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB3  | 13       | 0.68          |
| (1,345) | 1:1084:A:ILE:HD11 | 1:1087:A:TYR:HD1  | 12       | 0.67          |
| (1,345) | 1:1084:A:ILE:HD12 | 1:1087:A:TYR:HD1  | 12       | 0.67          |
| (1,345) | 1:1084:A:ILE:HD13 | 1:1087:A:TYR:HD1  | 12       | 0.67          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 13       | 0.67          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 13       | 0.67          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB2  | 5        | 0.67          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB3  | 5        | 0.67          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB2  | 5        | 0.67          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB3  | 5        | 0.67          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB2  | 15       | 0.66          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB3  | 15       | 0.66          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB2  | 15       | 0.66          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB3  | 15       | 0.66          |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H    | 9        | 0.65          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H    | 9        | 0.65          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H    | 9        | 0.65          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB2  | 11       | 0.65          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB3  | 11       | 0.65          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB2  | 11       | 0.65          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB3  | 11       | 0.65          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 11       | 0.64          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 11       | 0.64          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 11       | 0.64          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 11       | 0.64          |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H    | 20       | 0.63          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H    | 20       | 0.63          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H    | 20       | 0.63          |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H    | 13       | 0.61          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H    | 13       | 0.61          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H    | 13       | 0.61          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 7        | 0.61          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 2        | 0.6           |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 2        | 0.6           |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 13       | 0.58          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD11 | 3        | 0.58          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD12 | 3        | 0.58          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD13 | 3        | 0.58          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD11 | 3        | 0.58          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD12 | 3        | 0.58          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD13 | 3        | 0.58          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 2        | 0.58          |
| (1,450) | 1:1089:A:VAL:HG21 | 1:1091:A:PHE:H    | 11       | 0.57          |
| (1,450) | 1:1089:A:VAL:HG22 | 1:1091:A:PHE:H    | 11       | 0.57          |
| (1,450) | 1:1089:A:VAL:HG23 | 1:1091:A:PHE:H    | 11       | 0.57          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 1        | 0.57          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 14       | 0.56          |
| (1,133) | 1:1068:A:TYR:HD1  | 1:1069:A:VAL:HG11 | 11       | 0.56          |
| (1,133) | 1:1068:A:TYR:HD1  | 1:1069:A:VAL:HG12 | 11       | 0.56          |
| (1,133) | 1:1068:A:TYR:HD1  | 1:1069:A:VAL:HG13 | 11       | 0.56          |
| (1,133) | 1:1068:A:TYR:HD2  | 1:1069:A:VAL:HG11 | 11       | 0.56          |
| (1,133) | 1:1068:A:TYR:HD2  | 1:1069:A:VAL:HG12 | 11       | 0.56          |
| (1,133) | 1:1068:A:TYR:HD2  | 1:1069:A:VAL:HG13 | 11       | 0.56          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 3        | 0.56          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 4        | 0.55          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 6        | 0.55          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 9        | 0.55          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 10       | 0.55          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 15       | 0.55          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 20       | 0.55          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 2        | 0.54          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 5        | 0.54          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 7        | 0.54          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 8        | 0.54          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 12       | 0.54          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 16       | 0.54          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 18       | 0.54          |
| (1,46)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 5        | 0.54          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 1        | 0.53          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 11       | 0.53          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 17       | 0.53          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 19       | 0.53          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 18       | 0.53          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 18       | 0.53          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB2  | 14       | 0.53          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB3  | 14       | 0.53          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB2  | 14       | 0.53          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB3  | 14       | 0.53          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 9        | 0.52          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 9        | 0.52          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 9        | 0.52          |
| (1,153) | 1:1070:A:LEU:H    | 1:1070:A:LEU:HG   | 3        | 0.52          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 18       | 0.52          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 11       | 0.52          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 11       | 0.52          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 14       | 0.51          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 14       | 0.51          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 15       | 0.51          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 15       | 0.51          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 20       | 0.51          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 20       | 0.51          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 9        | 0.49          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 9        | 0.49          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 17       | 0.49          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 17       | 0.49          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 20       | 0.48          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 20       | 0.48          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 4        | 0.48          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 4        | 0.48          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 4        | 0.48          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 4        | 0.48          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 4        | 0.48          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 4        | 0.48          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 4        | 0.48          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 4        | 0.48          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 4        | 0.48          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 9        | 0.48          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 1        | 0.48          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 1        | 0.48          |
| (1,519) | 1:1096:A:LEU:HA   | 1:1097:A:LYS:H    | 2        | 0.47          |
| (1,386) | 1:1086:A:LEU:HA   | 1:1086:A:LEU:HD21 | 18       | 0.47          |
| (1,386) | 1:1086:A:LEU:HA   | 1:1086:A:LEU:HD22 | 18       | 0.47          |
| (1,386) | 1:1086:A:LEU:HA   | 1:1086:A:LEU:HD23 | 18       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 10       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 13       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 13       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 13       | 0.47          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 13       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 13       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 13       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 13       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 13       | 0.47          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 13       | 0.47          |
| (1,21)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 9        | 0.47          |
| (1,21)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 9        | 0.47          |
| (1,21)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 9        | 0.47          |
| (1,21)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 9        | 0.47          |
| (1,21)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 9        | 0.47          |
| (1,21)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 9        | 0.47          |
| (1,519) | 1:1096:A:LEU:HA   | 1:1097:A:LYS:H    | 8        | 0.46          |
| (1,519) | 1:1096:A:LEU:HA   | 1:1097:A:LYS:H    | 15       | 0.46          |
| (1,46)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 10       | 0.46          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 13       | 0.45          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 13       | 0.45          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 17       | 0.45          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 17       | 0.45          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 20       | 0.45          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 20       | 0.45          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 20       | 0.45          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 20       | 0.45          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 20       | 0.45          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 20       | 0.45          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 20       | 0.45          |
| (1,519) | 1:1096:A:LEU:HA   | 1:1097:A:LYS:H    | 5        | 0.44          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 3        | 0.44          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 3        | 0.44          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 3        | 0.44          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 3        | 0.44          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 3        | 0.44          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 3        | 0.44          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 6        | 0.44          |
| (1,46)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 11       | 0.44          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 5        | 0.44          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 5        | 0.44          |
| (1,41)  | 1:1062:A:LYS:H    | 1:1063:A:GLN:H    | 6        | 0.44          |
| (1,41)  | 1:1062:A:LYS:H    | 1:1063:A:GLN:H    | 16       | 0.44          |
| (1,519) | 1:1096:A:LEU:HA   | 1:1097:A:LYS:H    | 12       | 0.43          |
| (1,41)  | 1:1062:A:LYS:H    | 1:1063:A:GLN:H    | 19       | 0.43          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 9        | 0.42          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 9        | 0.42          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 18       | 0.42          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 18       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 15       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 15       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 15       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 15       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 15       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 15       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 15       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 15       | 0.42          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 15       | 0.42          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 2        | 0.42          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 2        | 0.42          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 15       | 0.41          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 15       | 0.41          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 15       | 0.41          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 15       | 0.41          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 15       | 0.41          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 15       | 0.41          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 12       | 0.41          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 12       | 0.41          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 12       | 0.4           |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 12       | 0.4           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 9        | 0.4           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 9        | 0.4           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 9        | 0.4           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 9        | 0.4           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 9        | 0.4           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 9        | 0.4           |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 3        | 0.4           |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 3        | 0.4           |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 3        | 0.4           |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 3        | 0.4           |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 2        | 0.39          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 2        | 0.39          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 9        | 0.39          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 9        | 0.39          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 8        | 0.39          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 8        | 0.39          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 8        | 0.39          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 8        | 0.39          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 8        | 0.39          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 8        | 0.39          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 14       | 0.39          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 14       | 0.39          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 14       | 0.39          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 14       | 0.39          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 14       | 0.39          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 14       | 0.39          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 14       | 0.39          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 14       | 0.39          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 14       | 0.39          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 6        | 0.39          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 6        | 0.39          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 6        | 0.39          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 6        | 0.39          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 6        | 0.39          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 6        | 0.39          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 19       | 0.38          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 19       | 0.38          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 19       | 0.38          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 19       | 0.38          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 4        | 0.38          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 4        | 0.38          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 6        | 0.38          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 6        | 0.38          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 8        | 0.38          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 8        | 0.38          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 12       | 0.38          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 12       | 0.38          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 11       | 0.38          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 11       | 0.38          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 11       | 0.38          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 11       | 0.38          |
| (1,21)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 15       | 0.38          |
| (1,21)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 15       | 0.38          |
| (1,21)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 15       | 0.38          |
| (1,21)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 15       | 0.38          |
| (1,21)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 15       | 0.38          |
| (1,21)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 15       | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 1        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 1        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 1        | 0.38          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 1        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 1        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 1        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 4        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 4        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 4        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 4        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 4        | 0.38          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 4        | 0.38          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 16       | 0.37          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 16       | 0.37          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 7        | 0.37          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 7        | 0.37          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG12 | 15       | 0.37          |
| (1,304) | 1:1082:A:ILE:H    | 1:1084:A:ILE:HG13 | 15       | 0.37          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 12       | 0.37          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 12       | 0.37          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 12       | 0.37          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 12       | 0.37          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 14       | 0.36          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 14       | 0.36          |
| (1,477) | 1:1092:A:PHE:H    | 1:1093:A:LYS:HB2  | 18       | 0.36          |
| (1,477) | 1:1092:A:PHE:H    | 1:1093:A:LYS:HB3  | 18       | 0.36          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 20       | 0.36          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 20       | 0.36          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 20       | 0.36          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 1        | 0.36          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 1        | 0.36          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 1        | 0.36          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 8        | 0.36          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 8        | 0.36          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 8        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 2        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 2        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 2        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 2        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 9        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 9        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 9        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 9        | 0.36          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 15       | 0.36          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 15       | 0.36          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 15       | 0.36          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 15       | 0.36          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 20       | 0.36          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 20       | 0.36          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 20       | 0.36          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 20       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 12       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 16       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 16       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 16       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 16       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 16       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 16       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 16       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 16       | 0.36          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 16       | 0.36          |
| (1,46)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 8        | 0.36          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 6        | 0.35          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 6        | 0.35          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 6        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 1        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 1        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 1        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 1        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 7        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 7        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 7        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 7        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 8        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 8        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 8        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 8        | 0.35          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 16       | 0.35          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 16       | 0.35          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 16       | 0.35          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 16       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 5        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 8        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 9        | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 19       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 19       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 19       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 19       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 19       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 19       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 19       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 19       | 0.35          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 19       | 0.35          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 7        | 0.35          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 7        | 0.35          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 13       | 0.35          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 13       | 0.35          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 5        | 0.34          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 5        | 0.34          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 20       | 0.34          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 20       | 0.34          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 19       | 0.34          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 19       | 0.34          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 19       | 0.34          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 19       | 0.34          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 19       | 0.34          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 19       | 0.34          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 5        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 5        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 5        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 5        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 6        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 6        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 6        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 6        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 10       | 0.34          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 10       | 0.34          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 10       | 0.34          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 10       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 17       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 17       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 17       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 17       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 17       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 17       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 17       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 17       | 0.34          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 17       | 0.34          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 5        | 0.34          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 5        | 0.34          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 14       | 0.33          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 14       | 0.33          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 14       | 0.33          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 14       | 0.33          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 19       | 0.33          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 19       | 0.33          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 19       | 0.33          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 19       | 0.33          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 6        | 0.33          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 6        | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 4        | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 4        | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 5        | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 5        | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 12       | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 12       | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 13       | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 13       | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 15       | 0.33          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 15       | 0.33          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 11       | 0.32          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 11       | 0.32          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 4        | 0.32          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 4        | 0.32          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 4        | 0.32          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 4        | 0.32          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 17       | 0.32          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 17       | 0.32          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 17       | 0.32          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 17       | 0.32          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 18       | 0.32          |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 18       | 0.32          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 18       | 0.32          |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 18       | 0.32          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 7        | 0.32          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 7        | 0.32          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 16       | 0.32          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 16       | 0.32          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 8        | 0.32          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 8        | 0.32          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 11       | 0.32          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 11       | 0.32          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 14       | 0.32          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 14       | 0.32          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 18       | 0.31          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 18       | 0.31          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 18       | 0.31          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 18       | 0.31          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 18       | 0.31          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 18       | 0.31          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 18       | 0.31          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 18       | 0.31          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 18       | 0.31          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 5        | 0.31          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 5        | 0.31          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 5        | 0.31          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 10       | 0.31          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 10       | 0.31          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 12       | 0.31          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 12       | 0.31          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 17       | 0.31          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 17       | 0.31          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 19       | 0.31          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 19       | 0.31          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD11 | 11       | 0.31          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD12 | 11       | 0.31          |
| (1,68)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD13 | 11       | 0.31          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD11 | 11       | 0.31          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD12 | 11       | 0.31          |
| (1,68)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD13 | 11       | 0.31          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 6        | 0.31          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 6        | 0.31          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 9        | 0.31          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 9        | 0.31          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 16       | 0.31          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 16       | 0.31          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 19       | 0.31          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 19       | 0.31          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 2        | 0.3           |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 2        | 0.3           |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 2        | 0.3           |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 11       | 0.3           |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 11       | 0.3           |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 11       | 0.3           |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 16       | 0.3           |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 16       | 0.3           |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 16       | 0.3           |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 3        | 0.3           |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 3        | 0.3           |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 2        | 0.3           |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 2        | 0.3           |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 2        | 0.3           |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 17       | 0.3           |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 17       | 0.3           |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 17       | 0.3           |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD21 | 9        | 0.3           |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD22 | 9        | 0.3           |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD23 | 9        | 0.3           |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD21 | 9        | 0.3           |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD22 | 9        | 0.3           |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD23 | 9        | 0.3           |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD21 | 9        | 0.3           |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD22 | 9        | 0.3           |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD23 | 9        | 0.3           |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA2  | 13       | 0.3           |
| (1,156) | 1:1070:A:LEU:HB2  | 1:1074:A:GLY:HA3  | 13       | 0.3           |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA2  | 13       | 0.3           |
| (1,156) | 1:1070:A:LEU:HB3  | 1:1074:A:GLY:HA3  | 13       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 6        | 0.3           |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 20       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 20       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 20       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 20       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 20       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 20       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 20       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 20       | 0.3           |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 20       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 2        | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 2        | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 3        | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 3        | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 9        | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 9        | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 13       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 13       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 14       | 0.3           |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 14       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 15       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 15       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 18       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 18       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 20       | 0.3           |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 20       | 0.3           |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 1        | 0.3           |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 1        | 0.3           |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 3        | 0.3           |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 3        | 0.3           |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 3        | 0.3           |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 3        | 0.3           |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 3        | 0.3           |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 3        | 0.3           |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 10       | 0.29          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 10       | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 9        | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 9        | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 9        | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 13       | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 13       | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 13       | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 14       | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 14       | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 14       | 0.29          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 17       | 0.29          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 17       | 0.29          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 3        | 0.29          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 3        | 0.29          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 3        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 7        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 7        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 7        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 7        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 7        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 7        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 7        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 7        | 0.29          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 7        | 0.29          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 1        | 0.29          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 1        | 0.29          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 8        | 0.29          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 8        | 0.29          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 11       | 0.29          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 11       | 0.29          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 7        | 0.29          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 7        | 0.29          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 18       | 0.29          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 18       | 0.29          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 20       | 0.29          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 20       | 0.29          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 17       | 0.29          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 8        | 0.29          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 8        | 0.29          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG11 | 12       | 0.28          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG12 | 12       | 0.28          |
| (1,443) | 1:1089:A:VAL:H    | 1:1089:A:VAL:HG13 | 12       | 0.28          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 14       | 0.28          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 14       | 0.28          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 12       | 0.28          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 12       | 0.28          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 12       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD21 | 15       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD22 | 15       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD23 | 15       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD21 | 15       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD22 | 15       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD23 | 15       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD21 | 15       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD22 | 15       | 0.28          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD23 | 15       | 0.28          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE1  | 4        | 0.28          |
| (1,87)  | 1:1065:A:LEU:HG   | 1:1068:A:TYR:HE2  | 4        | 0.28          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 2        | 0.28          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 2        | 0.28          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 1        | 0.27          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 1        | 0.27          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 12       | 0.27          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 12       | 0.27          |
| (1,528) | 1:1097:A:LYS:HB3  | 1:1098:A:GLU:H    | 7        | 0.27          |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 11       | 0.27          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 1        | 0.27          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 1        | 0.27          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 8        | 0.27          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 8        | 0.27          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 16       | 0.27          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 16       | 0.27          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 1        | 0.27          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 1        | 0.27          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 1        | 0.27          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 1        | 0.27          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 1        | 0.27          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 1        | 0.27          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 1        | 0.27          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 1        | 0.27          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 1        | 0.27          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 17       | 0.27          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 17       | 0.27          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 17       | 0.27          |
| (1,67)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 7        | 0.27          |
| (1,67)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 7        | 0.27          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 3        | 0.27          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 3        | 0.27          |
| (1,41)  | 1:1062:A:LYS:H    | 1:1063:A:GLN:H    | 4        | 0.27          |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 13       | 0.26          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 17       | 0.26          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 17       | 0.26          |
| (1,174) | 1:1072:A:GLY:HA2  | 1:1076:A:LEU:HD11 | 19       | 0.26          |
| (1,174) | 1:1072:A:GLY:HA2  | 1:1076:A:LEU:HD12 | 19       | 0.26          |
| (1,174) | 1:1072:A:GLY:HA2  | 1:1076:A:LEU:HD13 | 19       | 0.26          |
| (1,174) | 1:1072:A:GLY:HA2  | 1:1076:A:LEU:HD21 | 19       | 0.26          |
| (1,174) | 1:1072:A:GLY:HA2  | 1:1076:A:LEU:HD22 | 19       | 0.26          |
| (1,174) | 1:1072:A:GLY:HA2  | 1:1076:A:LEU:HD23 | 19       | 0.26          |
| (1,139) | 1:1069:A:VAL:H    | 1:1069:A:VAL:HG11 | 11       | 0.26          |
| (1,139) | 1:1069:A:VAL:H    | 1:1069:A:VAL:HG12 | 11       | 0.26          |
| (1,139) | 1:1069:A:VAL:H    | 1:1069:A:VAL:HG13 | 11       | 0.26          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 2        | 0.26          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 2        | 0.26          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 2        | 0.26          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 2        | 0.26          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 2        | 0.26          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 2        | 0.26          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 2        | 0.26          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 2        | 0.26          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 2        | 0.26          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 19       | 0.26          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 19       | 0.26          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 19       | 0.26          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 10       | 0.26          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 10       | 0.26          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 7        | 0.26          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 14       | 0.26          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 6        | 0.25          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 6        | 0.25          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 11       | 0.25          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 11       | 0.25          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 11       | 0.25          |
| (1,372) | 1:1086:A:LEU:HA   | 1:1086:A:LEU:HG   | 18       | 0.25          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 18       | 0.25          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 18       | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 6        | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 6        | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 6        | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 6        | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 6        | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 6        | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 11       | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 11       | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 11       | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 11       | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 11       | 0.25          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 11       | 0.25          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 7        | 0.25          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 7        | 0.25          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 7        | 0.25          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB2  | 17       | 0.25          |
| (1,63)  | 1:1063:A:GLN:H    | 1:1064:A:MET:HB3  | 17       | 0.25          |
| (1,41)  | 1:1062:A:LYS:H    | 1:1063:A:GLN:H    | 8        | 0.25          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 7        | 0.24          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 7        | 0.24          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG2  | 6        | 0.24          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG3  | 6        | 0.24          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 16       | 0.24          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 16       | 0.24          |
| (1,229) | 1:1077:A:LEU:H    | 1:1078:A:LEU:HD11 | 5        | 0.24          |
| (1,229) | 1:1077:A:LEU:H    | 1:1078:A:LEU:HD12 | 5        | 0.24          |
| (1,229) | 1:1077:A:LEU:H    | 1:1078:A:LEU:HD13 | 5        | 0.24          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,229) | 1:1077:A:LEU:H    | 1:1078:A:LEU:HD21 | 5        | 0.24          |
| (1,229) | 1:1077:A:LEU:H    | 1:1078:A:LEU:HD22 | 5        | 0.24          |
| (1,229) | 1:1077:A:LEU:H    | 1:1078:A:LEU:HD23 | 5        | 0.24          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 11       | 0.24          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 11       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 13       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 13       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 13       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 13       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 13       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 13       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 18       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 18       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 18       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 18       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 18       | 0.24          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 18       | 0.24          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE1  | 14       | 0.24          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE2  | 14       | 0.24          |
| (1,67)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 3        | 0.24          |
| (1,67)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 3        | 0.24          |
| (1,67)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 10       | 0.24          |
| (1,67)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 10       | 0.24          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 2        | 0.24          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 5        | 0.24          |
| (1,46)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 16       | 0.24          |
| (1,18)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:H    | 4        | 0.24          |
| (1,18)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:H    | 4        | 0.24          |
| (1,18)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:H    | 4        | 0.24          |
| (1,18)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:H    | 4        | 0.24          |
| (1,18)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:H    | 4        | 0.24          |
| (1,18)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:H    | 4        | 0.24          |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 1        | 0.23          |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 20       | 0.23          |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG11 | 10       | 0.23          |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG12 | 10       | 0.23          |
| (1,428) | 1:1088:A:LYS:H    | 1:1089:A:VAL:HG13 | 10       | 0.23          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 10       | 0.23          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 10       | 0.23          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 19       | 0.23          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 19       | 0.23          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 19       | 0.23          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 7        | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 7        | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 7        | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 7        | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 7        | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 7        | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 14       | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 14       | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 14       | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 14       | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 14       | 0.23          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 14       | 0.23          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 3        | 0.23          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 3        | 0.23          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 9        | 0.23          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 9        | 0.23          |
| (1,18)  | 1:1058:A:VAL:HG11 | 1:1060:A:TYR:H    | 8        | 0.23          |
| (1,18)  | 1:1058:A:VAL:HG12 | 1:1060:A:TYR:H    | 8        | 0.23          |
| (1,18)  | 1:1058:A:VAL:HG13 | 1:1060:A:TYR:H    | 8        | 0.23          |
| (1,18)  | 1:1058:A:VAL:HG21 | 1:1060:A:TYR:H    | 8        | 0.23          |
| (1,18)  | 1:1058:A:VAL:HG22 | 1:1060:A:TYR:H    | 8        | 0.23          |
| (1,18)  | 1:1058:A:VAL:HG23 | 1:1060:A:TYR:H    | 8        | 0.23          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 17       | 0.22          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 17       | 0.22          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 5        | 0.22          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 15       | 0.22          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 2        | 0.22          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 2        | 0.22          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 14       | 0.22          |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD11 | 3        | 0.22          |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD12 | 3        | 0.22          |
| (1,51)  | 1:1063:A:GLN:HG2  | 1:1065:A:LEU:HD13 | 3        | 0.22          |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 6        | 0.21          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG11 | 15       | 0.21          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG12 | 15       | 0.21          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG13 | 15       | 0.21          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG11 | 15       | 0.21          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG12 | 15       | 0.21          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG13 | 15       | 0.21          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG11 | 15       | 0.21          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG12 | 15       | 0.21          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG13 | 15       | 0.21          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 13       | 0.21          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 13       | 0.21          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 13       | 0.21          |
| (1,366) | 1:1085:A:VAL:H    | 1:1086:A:LEU:HG   | 8        | 0.21          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 4        | 0.21          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 4        | 0.21          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 4        | 0.21          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 12       | 0.21          |
| (1,532) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HB2  | 2        | 0.2           |
| (1,531) | 1:1097:A:LYS:HB2  | 1:1098:A:GLU:H    | 5        | 0.2           |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 15       | 0.2           |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 18       | 0.2           |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 3        | 0.2           |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 17       | 0.2           |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 20       | 0.2           |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 20       | 0.2           |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 20       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD21 | 12       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD22 | 12       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD23 | 12       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD21 | 12       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD22 | 12       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD23 | 12       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD21 | 12       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD22 | 12       | 0.2           |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD23 | 12       | 0.2           |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 8        | 0.2           |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 9        | 0.2           |
| (1,213) | 1:1076:A:LEU:HB2  | 1:1077:A:LEU:H    | 19       | 0.2           |
| (1,213) | 1:1076:A:LEU:HB3  | 1:1077:A:LEU:H    | 19       | 0.2           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 4        | 0.2           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 4        | 0.2           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 4        | 0.2           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 4        | 0.2           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 4        | 0.2           |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 4        | 0.2           |
| (1,90)  | 1:1065:A:LEU:HA   | 1:1065:A:LEU:HG   | 3        | 0.2           |
| (1,90)  | 1:1065:A:LEU:HA   | 1:1065:A:LEU:HG   | 11       | 0.2           |
| (1,90)  | 1:1065:A:LEU:HA   | 1:1065:A:LEU:HG   | 20       | 0.2           |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 10       | 0.2           |
| (1,21)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HD1  | 20       | 0.2           |
| (1,21)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HD2  | 20       | 0.2           |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,21)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HD1  | 20       | 0.2           |
| (1,21)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HD2  | 20       | 0.2           |
| (1,21)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HD1  | 20       | 0.2           |
| (1,21)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HD2  | 20       | 0.2           |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 15       | 0.19          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 15       | 0.19          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 18       | 0.19          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 18       | 0.19          |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 11       | 0.19          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 19       | 0.19          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 19       | 0.19          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG2  | 8        | 0.19          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG3  | 8        | 0.19          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG2  | 19       | 0.19          |
| (1,425) | 1:1087:A:TYR:HD1  | 1:1088:A:LYS:HG3  | 19       | 0.19          |
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 15       | 0.19          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 15       | 0.19          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 14       | 0.19          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 14       | 0.19          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 14       | 0.19          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD21 | 8        | 0.19          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD22 | 8        | 0.19          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD23 | 8        | 0.19          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD21 | 8        | 0.19          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD22 | 8        | 0.19          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD23 | 8        | 0.19          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD21 | 8        | 0.19          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD22 | 8        | 0.19          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD23 | 8        | 0.19          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 6        | 0.19          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 12       | 0.19          |
| (1,241) | 1:1078:A:LEU:HG   | 1:1082:A:ILE:HG12 | 5        | 0.19          |
| (1,241) | 1:1078:A:LEU:HG   | 1:1082:A:ILE:HG13 | 5        | 0.19          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 10       | 0.19          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 10       | 0.19          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 10       | 0.19          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 10       | 0.19          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 10       | 0.19          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 10       | 0.19          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 2        | 0.19          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 2        | 0.19          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 2        | 0.19          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 12       | 0.19          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 12       | 0.19          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 12       | 0.19          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 8        | 0.19          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 15       | 0.19          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 18       | 0.19          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 7        | 0.19          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 7        | 0.19          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 7        | 0.19          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 7        | 0.19          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 7        | 0.19          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 7        | 0.19          |
| (1,14)  | 1:1058:A:VAL:H    | 1:1058:A:VAL:HB   | 10       | 0.19          |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 12       | 0.18          |
| (1,484) | 1:1093:A:LYS:H    | 1:1093:A:LYS:HD2  | 18       | 0.18          |
| (1,484) | 1:1093:A:LYS:H    | 1:1093:A:LYS:HD3  | 18       | 0.18          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 12       | 0.18          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 12       | 0.18          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 13       | 0.18          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 13       | 0.18          |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 9        | 0.18          |
| (1,67)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 2        | 0.18          |
| (1,67)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 2        | 0.18          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 9        | 0.18          |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD11 | 17       | 0.18          |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD12 | 17       | 0.18          |
| (1,47)  | 1:1063:A:GLN:HG3  | 1:1065:A:LEU:HD13 | 17       | 0.18          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 4        | 0.17          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 4        | 0.17          |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 1        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 1        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 1        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 4        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 4        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 6        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 6        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 8        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 8        | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 11       | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 11       | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 16       | 0.17          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 16       | 0.17          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,411) | 1:1087:A:TYR:HE1  | 1:1088:A:LYS:H    | 4        | 0.17          |
| (1,411) | 1:1087:A:TYR:HE2  | 1:1088:A:LYS:H    | 4        | 0.17          |
| (1,375) | 1:1086:A:LEU:HG   | 1:1092:A:PHE:HE1  | 18       | 0.17          |
| (1,375) | 1:1086:A:LEU:HG   | 1:1092:A:PHE:HE2  | 18       | 0.17          |
| (1,366) | 1:1085:A:VAL:H    | 1:1086:A:LEU:HG   | 2        | 0.17          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 10       | 0.17          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE1  | 17       | 0.17          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE2  | 17       | 0.17          |
| (1,50)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 12       | 0.17          |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 5        | 0.16          |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 19       | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 3        | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 3        | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 7        | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 7        | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 9        | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 9        | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 10       | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 10       | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 17       | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 17       | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 20       | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 20       | 0.16          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 16       | 0.16          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 16       | 0.16          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 16       | 0.16          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD21 | 4        | 0.16          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD22 | 4        | 0.16          |
| (1,362) | 1:1085:A:VAL:HG11 | 1:1086:A:LEU:HD23 | 4        | 0.16          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD21 | 4        | 0.16          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD22 | 4        | 0.16          |
| (1,362) | 1:1085:A:VAL:HG12 | 1:1086:A:LEU:HD23 | 4        | 0.16          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD21 | 4        | 0.16          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD22 | 4        | 0.16          |
| (1,362) | 1:1085:A:VAL:HG13 | 1:1086:A:LEU:HD23 | 4        | 0.16          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 5        | 0.16          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 5        | 0.16          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 5        | 0.16          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 1        | 0.16          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 1        | 0.16          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD11 | 3        | 0.16          |
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD12 | 3        | 0.16          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,138) | 1:1069:A:VAL:HG11 | 1:1073:A:ILE:HD13 | 3        | 0.16          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD11 | 3        | 0.16          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD12 | 3        | 0.16          |
| (1,138) | 1:1069:A:VAL:HG12 | 1:1073:A:ILE:HD13 | 3        | 0.16          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD11 | 3        | 0.16          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD12 | 3        | 0.16          |
| (1,138) | 1:1069:A:VAL:HG13 | 1:1073:A:ILE:HD13 | 3        | 0.16          |
| (1,67)  | 1:1063:A:GLN:HG2  | 1:1064:A:MET:H    | 1        | 0.16          |
| (1,67)  | 1:1063:A:GLN:HG3  | 1:1064:A:MET:H    | 1        | 0.16          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB2  | 20       | 0.16          |
| (1,43)  | 1:1062:A:LYS:HB2  | 1:1064:A:MET:HB3  | 20       | 0.16          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB2  | 20       | 0.16          |
| (1,43)  | 1:1062:A:LYS:HB3  | 1:1064:A:MET:HB3  | 20       | 0.16          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 2        | 0.15          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 2        | 0.15          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD2  | 5        | 0.15          |
| (1,480) | 1:1093:A:LYS:HA   | 1:1093:A:LYS:HD3  | 5        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG11 | 4        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG12 | 4        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD21 | 1:1089:A:VAL:HG13 | 4        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG11 | 4        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG12 | 4        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD22 | 1:1089:A:VAL:HG13 | 4        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG11 | 4        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG12 | 4        | 0.15          |
| (1,400) | 1:1086:A:LEU:HD23 | 1:1089:A:VAL:HG13 | 4        | 0.15          |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG11 | 20       | 0.15          |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG12 | 20       | 0.15          |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG13 | 20       | 0.15          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 14       | 0.15          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 16       | 0.15          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 19       | 0.15          |
| (1,257) | 1:1079:A:LEU:HA   | 1:1083:A:PHE:H    | 20       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 5        | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 5        | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 5        | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 5        | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 7        | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 7        | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 7        | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 7        | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 11       | 0.15          |

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| Key     | Atom-1           | Atom-2            | Model ID | Violation (Å) |
|---------|------------------|-------------------|----------|---------------|
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 11       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 11       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 11       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 14       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 14       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 14       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 14       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 15       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 15       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 15       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 15       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 18       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 18       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 18       | 0.15          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 18       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 1        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 1        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 1        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG21 | 1        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG22 | 1        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG23 | 1        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 2        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 2        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 2        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG21 | 2        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG22 | 2        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG23 | 2        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 5        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 5        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 5        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG21 | 5        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG22 | 5        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG23 | 5        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 7        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 7        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 7        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG21 | 7        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG22 | 7        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG23 | 7        | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 14       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 14       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 14       | 0.15          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 14       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 14       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 14       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG21 | 15       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG22 | 15       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG23 | 15       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 15       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 15       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 15       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG21 | 17       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG22 | 17       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG23 | 17       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 17       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 17       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 17       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG21 | 18       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG22 | 18       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG23 | 18       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 18       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 18       | 0.15          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 18       | 0.15          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 6        | 0.15          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD1  | 6        | 0.15          |
| (1,45)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:HD2  | 6        | 0.15          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB2  | 2        | 0.15          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB3  | 2        | 0.15          |
| (1,14)  | 1:1058:A:VAL:H    | 1:1058:A:VAL:HB   | 17       | 0.15          |
| (1,540) | 1:1097:A:LYS:HB2  | 1:1098:A:GLU:H    | 7        | 0.14          |
| (1,540) | 1:1097:A:LYS:HB3  | 1:1098:A:GLU:H    | 7        | 0.14          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 3        | 0.14          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 3        | 0.14          |
| (1,526) | 1:1096:A:LEU:HD11 | 1:1097:A:LYS:HB2  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD11 | 1:1097:A:LYS:HB3  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD12 | 1:1097:A:LYS:HB2  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD12 | 1:1097:A:LYS:HB3  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD13 | 1:1097:A:LYS:HB2  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD13 | 1:1097:A:LYS:HB3  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD21 | 1:1097:A:LYS:HB2  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD21 | 1:1097:A:LYS:HB3  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD22 | 1:1097:A:LYS:HB2  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD22 | 1:1097:A:LYS:HB3  | 20       | 0.14          |
| (1,526) | 1:1096:A:LEU:HD23 | 1:1097:A:LYS:HB2  | 20       | 0.14          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,526) | 1:1096:A:LEU:HD23 | 1:1097:A:LYS:HB3  | 20       | 0.14          |
| (1,502) | 1:1094:A:ARG:HA   | 1:1094:A:ARG:HG2  | 7        | 0.14          |
| (1,502) | 1:1094:A:ARG:HA   | 1:1094:A:ARG:HG3  | 7        | 0.14          |
| (1,477) | 1:1092:A:PHE:H    | 1:1093:A:LYS:HB2  | 2        | 0.14          |
| (1,477) | 1:1092:A:PHE:H    | 1:1093:A:LYS:HB3  | 2        | 0.14          |
| (1,465) | 1:1091:A:PHE:H    | 1:1092:A:PHE:H    | 10       | 0.14          |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG11 | 9        | 0.14          |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG12 | 9        | 0.14          |
| (1,399) | 1:1086:A:LEU:HA   | 1:1089:A:VAL:HG13 | 9        | 0.14          |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD21 | 9        | 0.14          |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD22 | 9        | 0.14          |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD23 | 9        | 0.14          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 15       | 0.14          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 15       | 0.14          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 15       | 0.14          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 1        | 0.14          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 2        | 0.14          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 11       | 0.14          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 17       | 0.14          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 20       | 0.14          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 7        | 0.14          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 7        | 0.14          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 9        | 0.14          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 9        | 0.14          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 5        | 0.14          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 5        | 0.14          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 5        | 0.14          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 5        | 0.14          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 5        | 0.14          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 5        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 2        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 2        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 2        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 2        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 6        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 6        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 6        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 6        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 8        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 8        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 8        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 8        | 0.14          |

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| Key     | Atom-1           | Atom-2            | Model ID | Violation (Å) |
|---------|------------------|-------------------|----------|---------------|
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 9        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 9        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 9        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 9        | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 12       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 12       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 12       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 12       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 13       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 13       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 13       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 13       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 19       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 19       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 19       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 19       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 20       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 20       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 20       | 0.14          |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 20       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 6        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 6        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 6        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG21 | 6        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG22 | 6        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG23 | 6        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 8        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 8        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 8        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG21 | 8        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG22 | 8        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG23 | 8        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 9        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 9        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 9        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG21 | 9        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG22 | 9        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG23 | 9        | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG21 | 12       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG22 | 12       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2 | 1:1069:A:VAL:HG23 | 12       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3 | 1:1069:A:VAL:HG21 | 12       | 0.14          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 12       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 12       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG21 | 16       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG22 | 16       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG23 | 16       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 16       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 16       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 16       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG21 | 19       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG22 | 19       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG23 | 19       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 19       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 19       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 19       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG21 | 20       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG22 | 20       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG23 | 20       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 20       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 20       | 0.14          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 20       | 0.14          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 1        | 0.14          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 1        | 0.14          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 1        | 0.14          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 16       | 0.14          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB2  | 5        | 0.14          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB3  | 5        | 0.14          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB2  | 8        | 0.14          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB3  | 8        | 0.14          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB2  | 13       | 0.14          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB3  | 13       | 0.14          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE1  | 17       | 0.14          |
| (1,20)  | 1:1059:A:VAL:HG21 | 1:1060:A:TYR:HE2  | 17       | 0.14          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE1  | 17       | 0.14          |
| (1,20)  | 1:1059:A:VAL:HG22 | 1:1060:A:TYR:HE2  | 17       | 0.14          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE1  | 17       | 0.14          |
| (1,20)  | 1:1059:A:VAL:HG23 | 1:1060:A:TYR:HE2  | 17       | 0.14          |
| (1,531) | 1:1097:A:LYS:HB2  | 1:1098:A:GLU:H    | 19       | 0.13          |
| (1,409) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HE1  | 13       | 0.13          |
| (1,409) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HE2  | 13       | 0.13          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 7        | 0.13          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 13       | 0.13          |
| (1,222) | 1:1077:A:LEU:HB2  | 1:1078:A:LEU:H    | 8        | 0.13          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,222) | 1:1077:A:LEU:HB3  | 1:1078:A:LEU:H    | 8        | 0.13          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD11 | 17       | 0.13          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD12 | 17       | 0.13          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD13 | 17       | 0.13          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD21 | 17       | 0.13          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD22 | 17       | 0.13          |
| (1,176) | 1:1072:A:GLY:HA3  | 1:1076:A:LEU:HD23 | 17       | 0.13          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 4        | 0.13          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 4        | 0.13          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 4        | 0.13          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 4        | 0.13          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 16       | 0.13          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 16       | 0.13          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 16       | 0.13          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 16       | 0.13          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE1  | 9        | 0.13          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE2  | 9        | 0.13          |
| (1,409) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HE1  | 5        | 0.12          |
| (1,409) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HE2  | 5        | 0.12          |
| (1,409) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HE1  | 18       | 0.12          |
| (1,409) | 1:1087:A:TYR:H    | 1:1087:A:TYR:HE2  | 18       | 0.12          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 5        | 0.12          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 5        | 0.12          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 5        | 0.12          |
| (1,366) | 1:1085:A:VAL:H    | 1:1086:A:LEU:HG   | 7        | 0.12          |
| (1,354) | 1:1084:A:ILE:H    | 1:1086:A:LEU:H    | 18       | 0.12          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 18       | 0.12          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG12 | 10       | 0.12          |
| (1,161) | 1:1070:A:LEU:HB2  | 1:1073:A:ILE:HG13 | 10       | 0.12          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG12 | 10       | 0.12          |
| (1,161) | 1:1070:A:LEU:HB3  | 1:1073:A:ILE:HG13 | 10       | 0.12          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE1  | 1        | 0.12          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE2  | 1        | 0.12          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE1  | 5        | 0.12          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE2  | 5        | 0.12          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 9        | 0.12          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 9        | 0.12          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 9        | 0.12          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 18       | 0.12          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 18       | 0.12          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 18       | 0.12          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 3        | 0.12          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 11       | 0.12          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 19       | 0.12          |
| (1,37)  | 1:1060:A:TYR:H    | 1:1061:A:GLU:H    | 18       | 0.12          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB2  | 15       | 0.12          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB3  | 15       | 0.12          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB2  | 17       | 0.12          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB3  | 17       | 0.12          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD2  | 6        | 0.11          |
| (1,535) | 1:1097:A:LYS:H    | 1:1097:A:LYS:HD3  | 6        | 0.11          |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 3        | 0.11          |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 10       | 0.11          |
| (1,508) | 1:1095:A:ASN:HA   | 1:1095:A:ASN:HD22 | 14       | 0.11          |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD21 | 8        | 0.11          |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD22 | 8        | 0.11          |
| (1,395) | 1:1086:A:LEU:H    | 1:1086:A:LEU:HD23 | 8        | 0.11          |
| (1,380) | 1:1086:A:LEU:HD11 | 1:1091:A:PHE:H    | 7        | 0.11          |
| (1,380) | 1:1086:A:LEU:HD12 | 1:1091:A:PHE:H    | 7        | 0.11          |
| (1,380) | 1:1086:A:LEU:HD13 | 1:1091:A:PHE:H    | 7        | 0.11          |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG21 | 20       | 0.11          |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG22 | 20       | 0.11          |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG23 | 20       | 0.11          |
| (1,290) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HG   | 3        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 1        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 1        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 1        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 4        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 4        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 4        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 8        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 8        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 8        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 9        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 9        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 9        | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 10       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 10       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 10       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 15       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 15       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 15       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 16       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 16       | 0.11          |

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| Key     | Atom-1            | Atom-2            | Model ID | Violation (Å) |
|---------|-------------------|-------------------|----------|---------------|
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 16       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 19       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD22 | 19       | 0.11          |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD23 | 19       | 0.11          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB2  | 10       | 0.11          |
| (1,249) | 1:1079:A:LEU:HG   | 1:1083:A:PHE:HB3  | 10       | 0.11          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB2  | 10       | 0.11          |
| (1,188) | 1:1073:A:ILE:HA   | 1:1077:A:LEU:HB3  | 10       | 0.11          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG21 | 3        | 0.11          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG22 | 3        | 0.11          |
| (1,134) | 1:1068:A:TYR:HB2  | 1:1069:A:VAL:HG23 | 3        | 0.11          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG21 | 3        | 0.11          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG22 | 3        | 0.11          |
| (1,134) | 1:1068:A:TYR:HB3  | 1:1069:A:VAL:HG23 | 3        | 0.11          |
| (1,129) | 1:1068:A:TYR:HE1  | 1:1069:A:VAL:HB   | 11       | 0.11          |
| (1,129) | 1:1068:A:TYR:HE2  | 1:1069:A:VAL:HB   | 11       | 0.11          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE1  | 15       | 0.11          |
| (1,107) | 1:1066:A:TYR:H    | 1:1066:A:TYR:HE2  | 15       | 0.11          |
| (1,100) | 1:1065:A:LEU:HD11 | 1:1068:A:TYR:HB2  | 9        | 0.11          |
| (1,100) | 1:1065:A:LEU:HD11 | 1:1068:A:TYR:HB3  | 9        | 0.11          |
| (1,100) | 1:1065:A:LEU:HD12 | 1:1068:A:TYR:HB2  | 9        | 0.11          |
| (1,100) | 1:1065:A:LEU:HD12 | 1:1068:A:TYR:HB3  | 9        | 0.11          |
| (1,100) | 1:1065:A:LEU:HD13 | 1:1068:A:TYR:HB2  | 9        | 0.11          |
| (1,100) | 1:1065:A:LEU:HD13 | 1:1068:A:TYR:HB3  | 9        | 0.11          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD11 | 16       | 0.11          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD12 | 16       | 0.11          |
| (1,92)  | 1:1065:A:LEU:H    | 1:1065:A:LEU:HD13 | 16       | 0.11          |
| (1,60)  | 1:1063:A:GLN:HB2  | 1:1066:A:TYR:H    | 1        | 0.11          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB2  | 4        | 0.11          |
| (1,26)  | 1:1059:A:VAL:HA   | 1:1060:A:TYR:HB3  | 4        | 0.11          |
| (1,551) | 1:1099:A:LYS:H    | 1:1099:A:LYS:HD2  | 12       | 0.1           |
| (1,551) | 1:1099:A:LYS:H    | 1:1099:A:LYS:HD3  | 12       | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG21 | 4        | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG22 | 4        | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG23 | 4        | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG21 | 12       | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG22 | 12       | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG23 | 12       | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG21 | 15       | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG22 | 15       | 0.1           |
| (1,347) | 1:1084:A:ILE:H    | 1:1084:A:ILE:HG23 | 15       | 0.1           |
| (1,284) | 1:1081:A:LEU:H    | 1:1081:A:LEU:HD21 | 12       | 0.1           |

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| Key     | Atom-1           | Atom-2            | Model ID | Violation (Å) |
|---------|------------------|-------------------|----------|---------------|
| (1,284) | 1:1081:A:LEU:H   | 1:1081:A:LEU:HD22 | 12       | 0.1           |
| (1,284) | 1:1081:A:LEU:H   | 1:1081:A:LEU:HD23 | 12       | 0.1           |
| (1,284) | 1:1081:A:LEU:H   | 1:1081:A:LEU:HD21 | 14       | 0.1           |
| (1,284) | 1:1081:A:LEU:H   | 1:1081:A:LEU:HD22 | 14       | 0.1           |
| (1,284) | 1:1081:A:LEU:H   | 1:1081:A:LEU:HD23 | 14       | 0.1           |
| (1,284) | 1:1081:A:LEU:H   | 1:1081:A:LEU:HD21 | 17       | 0.1           |
| (1,284) | 1:1081:A:LEU:H   | 1:1081:A:LEU:HD22 | 17       | 0.1           |
| (1,284) | 1:1081:A:LEU:H   | 1:1081:A:LEU:HD23 | 17       | 0.1           |
| (1,176) | 1:1072:A:GLY:HA3 | 1:1076:A:LEU:HD11 | 2        | 0.1           |
| (1,176) | 1:1072:A:GLY:HA3 | 1:1076:A:LEU:HD12 | 2        | 0.1           |
| (1,176) | 1:1072:A:GLY:HA3 | 1:1076:A:LEU:HD13 | 2        | 0.1           |
| (1,176) | 1:1072:A:GLY:HA3 | 1:1076:A:LEU:HD21 | 2        | 0.1           |
| (1,176) | 1:1072:A:GLY:HA3 | 1:1076:A:LEU:HD22 | 2        | 0.1           |
| (1,176) | 1:1072:A:GLY:HA3 | 1:1076:A:LEU:HD23 | 2        | 0.1           |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 1        | 0.1           |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 1        | 0.1           |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 1        | 0.1           |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 1        | 0.1           |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG12 | 17       | 0.1           |
| (1,161) | 1:1070:A:LEU:HB2 | 1:1073:A:ILE:HG13 | 17       | 0.1           |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG12 | 17       | 0.1           |
| (1,161) | 1:1070:A:LEU:HB3 | 1:1073:A:ILE:HG13 | 17       | 0.1           |
| (1,88)  | 1:1065:A:LEU:H   | 1:1065:A:LEU:HG   | 10       | 0.1           |
| (1,60)  | 1:1063:A:GLN:HB2 | 1:1066:A:TYR:H    | 13       | 0.1           |
| (1,60)  | 1:1063:A:GLN:HB2 | 1:1066:A:TYR:H    | 20       | 0.1           |
| (1,43)  | 1:1062:A:LYS:HB2 | 1:1064:A:MET:HB2  | 17       | 0.1           |
| (1,43)  | 1:1062:A:LYS:HB2 | 1:1064:A:MET:HB3  | 17       | 0.1           |
| (1,43)  | 1:1062:A:LYS:HB3 | 1:1064:A:MET:HB2  | 17       | 0.1           |
| (1,43)  | 1:1062:A:LYS:HB3 | 1:1064:A:MET:HB3  | 17       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found