



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 PM UTC

PDB ID : 5IZB / pdb\_00005izb  
BMRB ID : 30042  
Title : Murin CXCL13 solution structure featuring a folded N-terminal domain  
Authors : Monneau, Y.R.; Lortat-Jacob, H.  
Deposited on : 2016-03-25

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

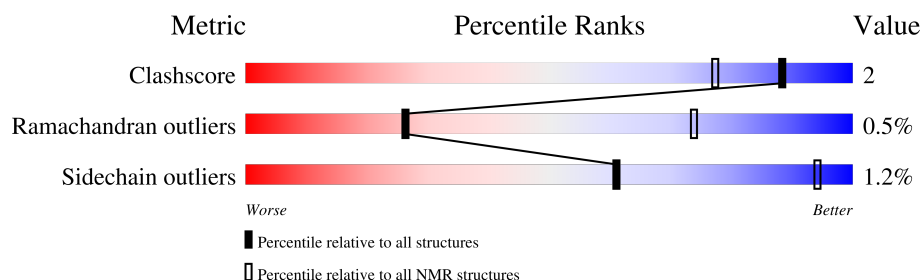
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 83%.

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     | 89     |  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:1-A:71 (71)         | 1.11              | 9            |

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1441 atoms, of which 748 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-X-C motif chemokine 13.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 89       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1441  | 437 | 748 | 132 | 118 | 6 |       |

There is a discrepancy between the modelled and reference sequences:

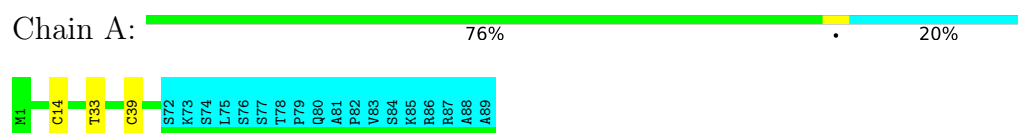
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 1       | MET      | -      | initiating methionine | UNP O55038 |

## 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: C-X-C motif chemokine 13

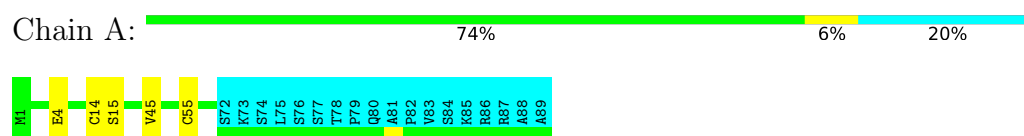


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

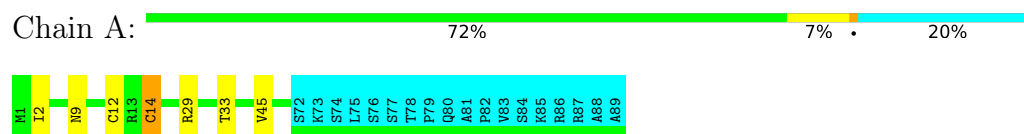
#### 4.2.1 Score per residue for model 1

- Molecule 1: C-X-C motif chemokine 13



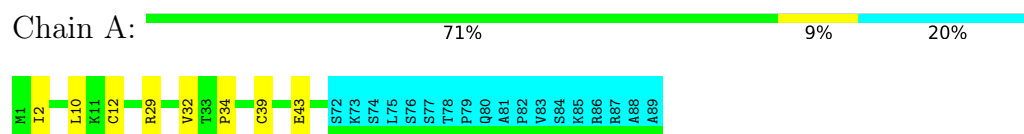
#### 4.2.2 Score per residue for model 2

- Molecule 1: C-X-C motif chemokine 13



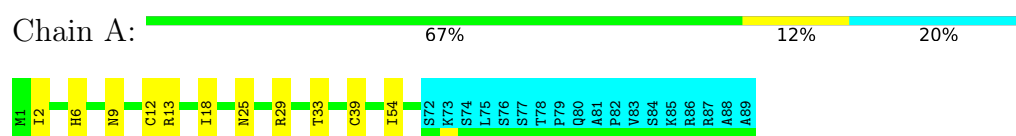
### 4.2.3 Score per residue for model 3

- Molecule 1: C-X-C motif chemokine 13



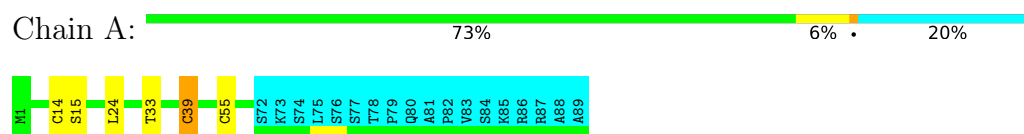
### 4.2.4 Score per residue for model 4

- Molecule 1: C-X-C motif chemokine 13



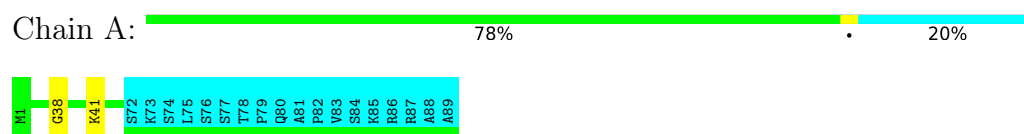
### 4.2.5 Score per residue for model 5

- Molecule 1: C-X-C motif chemokine 13



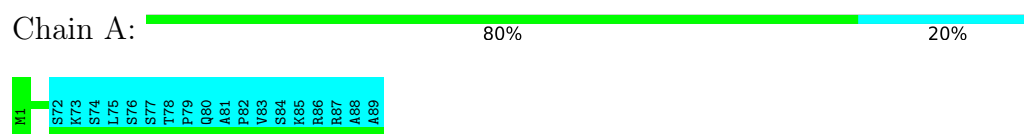
### 4.2.6 Score per residue for model 6

- Molecule 1: C-X-C motif chemokine 13



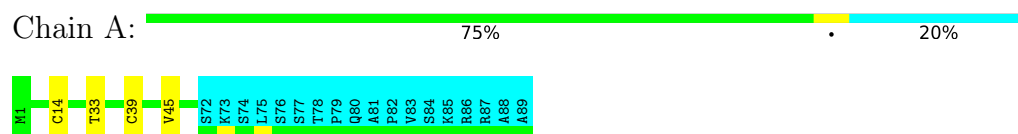
### 4.2.7 Score per residue for model 7

- Molecule 1: C-X-C motif chemokine 13



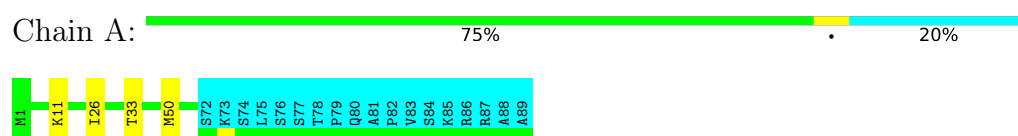
### 4.2.8 Score per residue for model 8

- Molecule 1: C-X-C motif chemokine 13



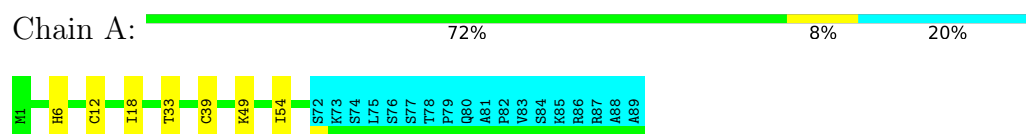
### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: C-X-C motif chemokine 13



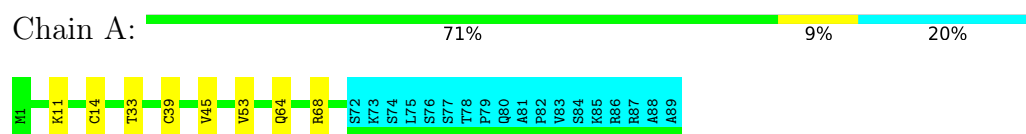
### 4.2.10 Score per residue for model 10

- Molecule 1: C-X-C motif chemokine 13



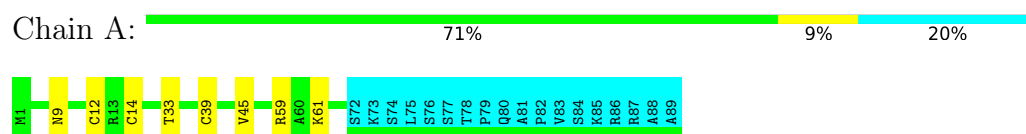
### 4.2.11 Score per residue for model 11

- Molecule 1: C-X-C motif chemokine 13



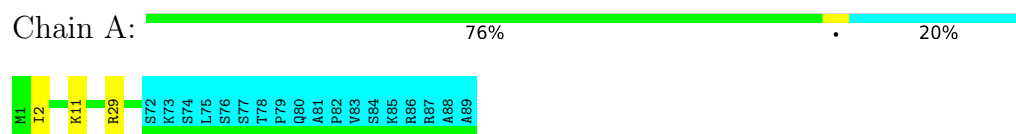
### 4.2.12 Score per residue for model 12

- Molecule 1: C-X-C motif chemokine 13



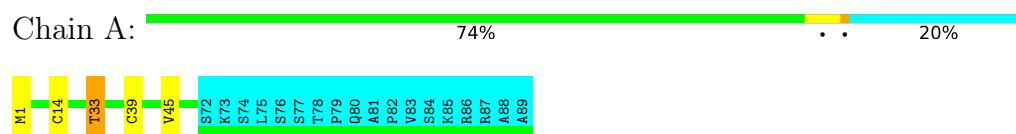
### 4.2.13 Score per residue for model 13

- Molecule 1: C-X-C motif chemokine 13



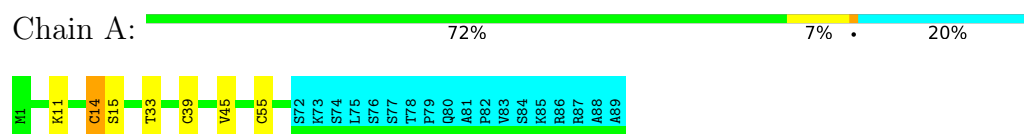
### 4.2.14 Score per residue for model 14

- Molecule 1: C-X-C motif chemokine 13



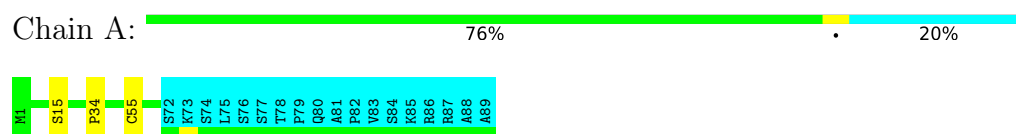
### 4.2.15 Score per residue for model 15

- Molecule 1: C-X-C motif chemokine 13



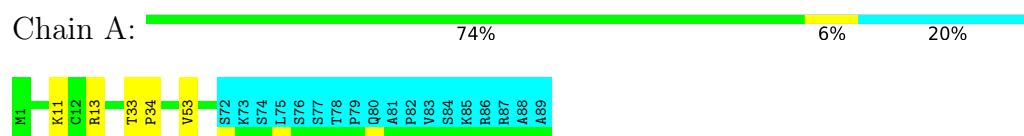
### 4.2.16 Score per residue for model 16

- Molecule 1: C-X-C motif chemokine 13



### 4.2.17 Score per residue for model 17

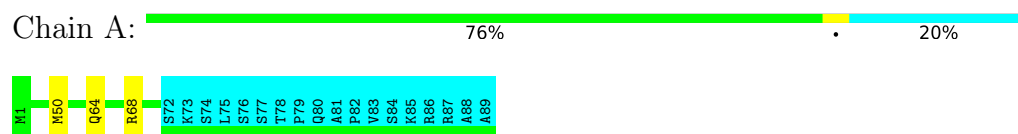
- Molecule 1: C-X-C motif chemokine 13





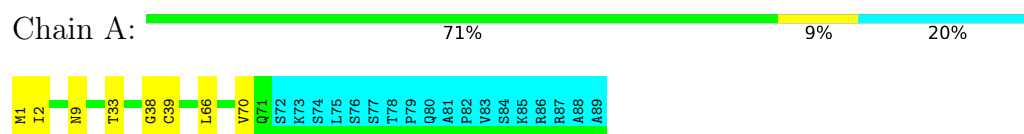
#### 4.2.18 Score per residue for model 18

- Molecule 1: C-X-C motif chemokine 13



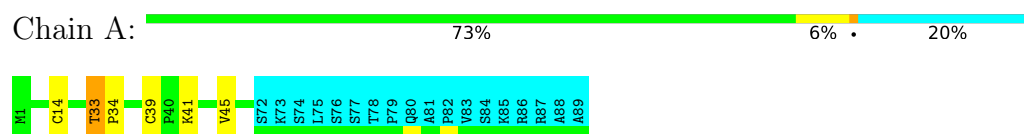
#### 4.2.19 Score per residue for model 19

- Molecule 1: C-X-C motif chemokine 13



#### 4.2.20 Score per residue for model 20

- Molecule 1: C-X-C motif chemokine 13



## 5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CYANA         | structure calculation |         |
| 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                       | 1047           |
| Number of shifts mapped to atoms             | 1047           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 83%            |

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.33±0.04    | 0±1/573 ( 0.1± 0.1%) | 0.87±0.04   | 0±0/778 ( 0.0± 0.1%) |
| All | All   | 1.33         | 10/11460 ( 0.1%)     | 0.88        | 2/15560 ( 0.0%)      |

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

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 34  | PRO  | CA-C  | 6.79 | 1.55        | 1.51     | 17     | 4     |
| 1   | A     | 33  | THR  | C-N   | 5.84 | 1.38        | 1.33     | 17     | 3     |
| 1   | A     | 2   | ILE  | CA-CB | 5.41 | 1.60        | 1.54     | 19     | 1     |
| 1   | A     | 53  | VAL  | CA-CB | 5.41 | 1.59        | 1.53     | 11     | 1     |
| 1   | A     | 32  | VAL  | CA-CB | 5.08 | 1.59        | 1.53     | 3      | 1     |

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

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | A     | 33  | THR  | CA-C-N | 5.25 | 123.44      | 119.66   | 20     | 1     |
| 1   | A     | 33  | THR  | C-N-CA | 5.25 | 123.44      | 119.66   | 20     | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 562   | 607      | 605      | 2±1     |
| All | All   | 11240 | 12140    | 12100    | 44      |

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 2.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:33:THR:HB   | 1:A:39:CYS:SG   | 0.67     | 2.29        | 19     | 7     |
| 1:A:12:CYS:SG   | 1:A:33:THR:HG21 | 0.67     | 2.29        | 4      | 4     |
| 1:A:14:CYS:SG   | 1:A:45:VAL:HG22 | 0.57     | 2.39        | 11     | 8     |
| 1:A:15:SER:N    | 1:A:55:CYS:SG   | 0.52     | 2.82        | 16     | 4     |
| 1:A:12:CYS:N    | 1:A:39:CYS:SG   | 0.47     | 2.88        | 3      | 2     |
| 1:A:9:ASN:ND2   | 1:A:12:CYS:SG   | 0.46     | 2.89        | 2      | 1     |
| 1:A:2:ILE:HB    | 1:A:29:ARG:HG2  | 0.45     | 1.88        | 2      | 4     |
| 1:A:13:ARG:HA   | 1:A:13:ARG:NE   | 0.45     | 2.27        | 4      | 1     |
| 1:A:18:ILE:HD12 | 1:A:54:ILE:HG23 | 0.45     | 1.89        | 4      | 2     |
| 1:A:64:GLN:O    | 1:A:68:ARG:HG2  | 0.44     | 2.13        | 11     | 2     |
| 1:A:6:HIS:CE1   | 1:A:12:CYS:SG   | 0.44     | 3.11        | 10     | 1     |
| 1:A:9:ASN:H     | 1:A:38:GLY:HA2  | 0.42     | 1.75        | 19     | 1     |
| 1:A:6:HIS:NE2   | 1:A:39:CYS:SG   | 0.42     | 2.92        | 10     | 1     |
| 1:A:13:ARG:NE   | 1:A:53:VAL:HG11 | 0.42     | 2.29        | 17     | 1     |
| 1:A:50:MET:SD   | 1:A:50:MET:N    | 0.42     | 2.92        | 18     | 1     |
| 1:A:9:ASN:N     | 1:A:39:CYS:SG   | 0.42     | 2.93        | 12     | 1     |
| 1:A:26:ILE:HB   | 1:A:50:MET:HE1  | 0.41     | 1.92        | 9      | 1     |
| 1:A:66:LEU:O    | 1:A:70:VAL:HG13 | 0.41     | 2.15        | 19     | 1     |
| 1:A:1:MET:SD    | 1:A:1:MET:N     | 0.40     | 2.94        | 19     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|------------|-------------|----|
| 1   | A     | 70/89 (79%)     | 65±2 (92±2%) | 5±2 (7±2%) | 0±0 (0±1%) | 26          | 74 |
| All | All   | 1400/1780 (79%) | 1295 (92%)   | 98 (7%)    | 7 (0%)     | 26          | 74 |

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 11  | LYS  | 4              |
| 1   | A     | 10  | LEU  | 1              |
| 1   | A     | 9   | ASN  | 1              |
| 1   | A     | 38  | GLY  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1   | A     | 65/80 (81%)     | 64±1 (99±1%) | 1±1 (1±1%) | 61          | 94 |
| All | All   | 1300/1600 (81%) | 1284 (99%)   | 16 (1%)    | 61          | 94 |

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     | 14  | CYS  | 3              |
| 1   | A     | 41  | LYS  | 2              |
| 1   | A     | 4   | GLU  | 1              |
| 1   | A     | 43  | GLU  | 1              |
| 1   | A     | 6   | HIS  | 1              |
| 1   | A     | 25  | ASN  | 1              |
| 1   | A     | 24  | LEU  | 1              |
| 1   | A     | 39  | CYS  | 1              |
| 1   | A     | 49  | LYS  | 1              |
| 1   | A     | 59  | ARG  | 1              |
| 1   | A     | 61  | LYS  | 1              |
| 1   | A     | 1   | MET  | 1              |
| 1   | A     | 11  | LYS  | 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *x13\_31.bmrB*

#### 7.1.1 Bookkeeping [i](#)

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1047 |
| Number of shifts mapped to atoms        | 1047 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 2    |

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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 85       | $-0.02 \pm 0.15$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 81       | $0.07 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 81       | $-0.02 \pm 0.73$                | None needed ( $< 0.5$ ppm) |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 858 atoms were assigned a chemical shift out of a possible 1030. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 269/351 (77%) | 137/142 (96%) | 67/142 (47%)    | 65/67 (97%)     |
| Sidechain | 549/630 (87%) | 375/413 (91%) | 167/189 (88%)   | 7/28 (25%)      |

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|          | <b>Total</b>   | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 40/49 (82%)    | 20/24 (83%)          | 18/19 (95%)           | 2/6 (33%)             |
| Overall  | 858/1030 (83%) | 532/579 (92%)        | 252/350 (72%)         | 74/101 (73%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1046 atoms were assigned a chemical shift out of a possible 1262. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 337/437 (77%)   | 171/176 (97%)        | 85/178 (48%)          | 81/83 (98%)           |
| Sidechain | 669/776 (86%)   | 455/508 (90%)        | 206/231 (89%)         | 8/37 (22%)            |
| Aromatic  | 40/49 (82%)     | 20/24 (83%)          | 18/19 (95%)           | 2/6 (33%)             |
| Overall   | 1046/1262 (83%) | 646/708 (91%)        | 309/428 (72%)         | 91/126 (72%)          |

#### 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.

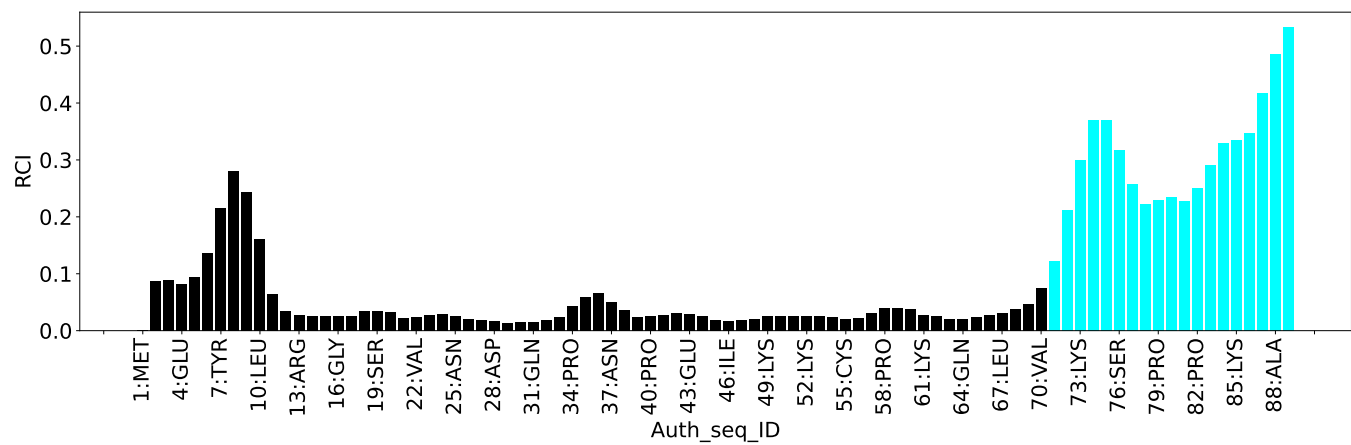
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 48  | THR  | HG1  | 5.89       | 0.08 – 2.19         | 22.5    |
| 1       | A     | 13  | ARG  | H    | 11.43      | 5.25 – 11.22        | 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                                | 1135  |
| Intra-residue ( $ i-j =0$ )                              | 303   |
| Sequential ( $ i-j =1$ )                                 | 251   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 194   |
| Long range ( $ i-j \geq 5$ )                             | 347   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 38    |
| Disulfide bond restraints                                | 2     |
| Total dihedral-angle restraints                          | 110   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 14.0  |
| Number of long range restraints per residue <sup>1</sup> | 4.2   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 21.1                                   | 0.2     |
| 0.2-0.5 (Medium) | 7.8                                    | 0.5     |
| >0.5 (Large)     | 2.5                                    | 2.08    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 13.8                                   | 8.31    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

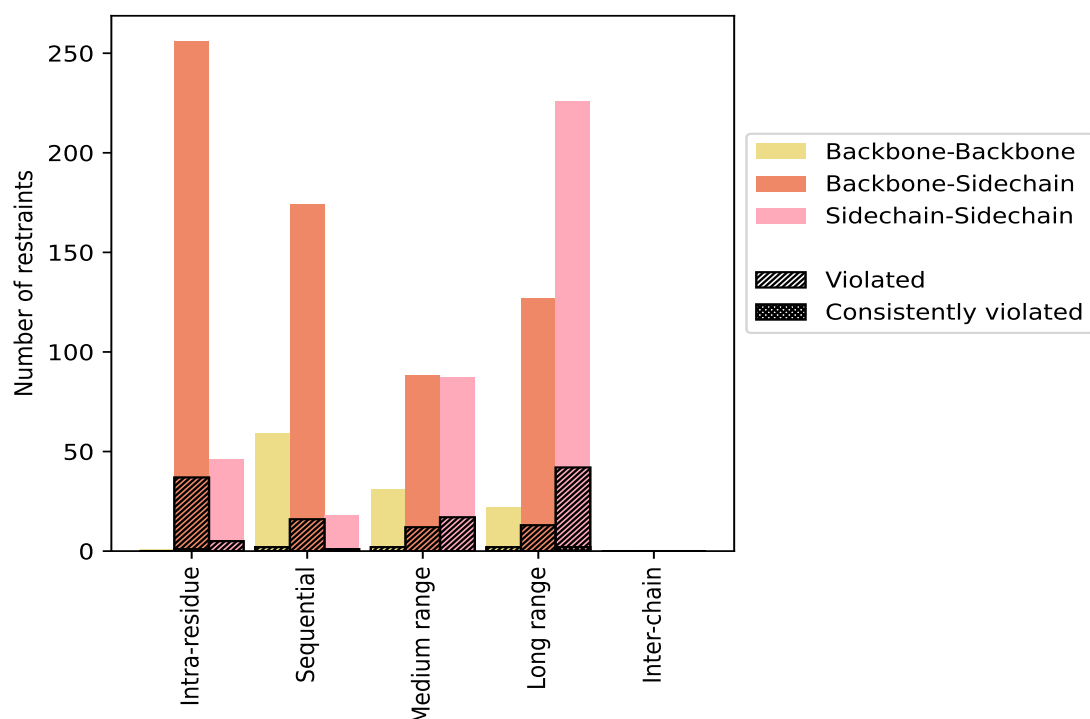
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>303</b>  | <b>26.7</b>    | <b>42</b>             | <b>13.9</b>    | <b>3.7</b>     | <b>1</b>                           | <b>0.3</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 1           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 256         | 22.6           | 37                    | 14.5           | 3.3            | 1                                  | 0.4            | 0.1            |
| Sidechain-Sidechain                                                         | 46          | 4.1            | 5                     | 10.9           | 0.4            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>251</b>  | <b>22.1</b>    | <b>19</b>             | <b>7.6</b>     | <b>1.7</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 59          | 5.2            | 2                     | 3.4            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 174         | 15.3           | 16                    | 9.2            | 1.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 18          | 1.6            | 1                     | 5.6            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>194</b>  | <b>17.1</b>    | <b>29</b>             | <b>14.9</b>    | <b>2.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 31          | 2.7            | 2                     | 6.5            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 76          | 6.7            | 10                    | 13.2           | 0.9            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 87          | 7.7            | 17                    | 19.5           | 1.5            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>347</b>  | <b>30.6</b>    | <b>54</b>             | <b>15.6</b>    | <b>4.8</b>     | <b>2</b>                           | <b>0.6</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 22          | 1.9            | 2                     | 9.1            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 101         | 8.9            | 10                    | 9.9            | 0.9            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 224         | 19.7           | 42                    | 18.8           | 3.7            | 2                                  | 0.9            | 0.2            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>38</b>   | <b>3.3</b>     | <b>5</b>              | <b>13.2</b>    | <b>0.4</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>2</b>    | <b>0.2</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>1135</b> | <b>100.0</b>   | <b>149</b>            | <b>13.1</b>    | <b>13.1</b>    | <b>3</b>                           | <b>0.3</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 113         | 10.0           | 6                     | 5.3            | 0.5            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 645         | 56.8           | 78                    | 12.1           | 6.9            | 1                                  | 0.2            | 0.1            |
| Sidechain-Sidechain                                                         | 377         | 33.2           | 65                    | 17.2           | 5.7            | 2                                  | 0.5            | 0.2            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 8                    | 1               | 5               | 14              | 0               | 28    | 0.19     | 0.69    | 0.12                | 0.16       |
| 2        | 12                   | 1               | 10              | 14              | 0               | 37    | 0.36     | 2.08    | 0.44                | 0.15       |
| 3        | 10                   | 4               | 6               | 15              | 0               | 35    | 0.2      | 0.94    | 0.17                | 0.14       |
| 4        | 7                    | 4               | 6               | 6               | 0               | 23    | 0.2      | 0.64    | 0.12                | 0.16       |
| 5        | 9                    | 2               | 5               | 13              | 0               | 29    | 0.23     | 0.62    | 0.15                | 0.16       |
| 6        | 7                    | 1               | 4               | 15              | 0               | 27    | 0.23     | 0.65    | 0.14                | 0.18       |
| 7        | 9                    | 2               | 6               | 14              | 0               | 31    | 0.18     | 0.54    | 0.09                | 0.15       |
| 8        | 8                    | 0               | 9               | 15              | 0               | 32    | 0.24     | 0.97    | 0.2                 | 0.18       |
| 9        | 4                    | 2               | 8               | 16              | 0               | 30    | 0.2      | 0.94    | 0.15                | 0.16       |
| 10       | 8                    | 3               | 12              | 18              | 0               | 41    | 0.27     | 1.39    | 0.31                | 0.16       |

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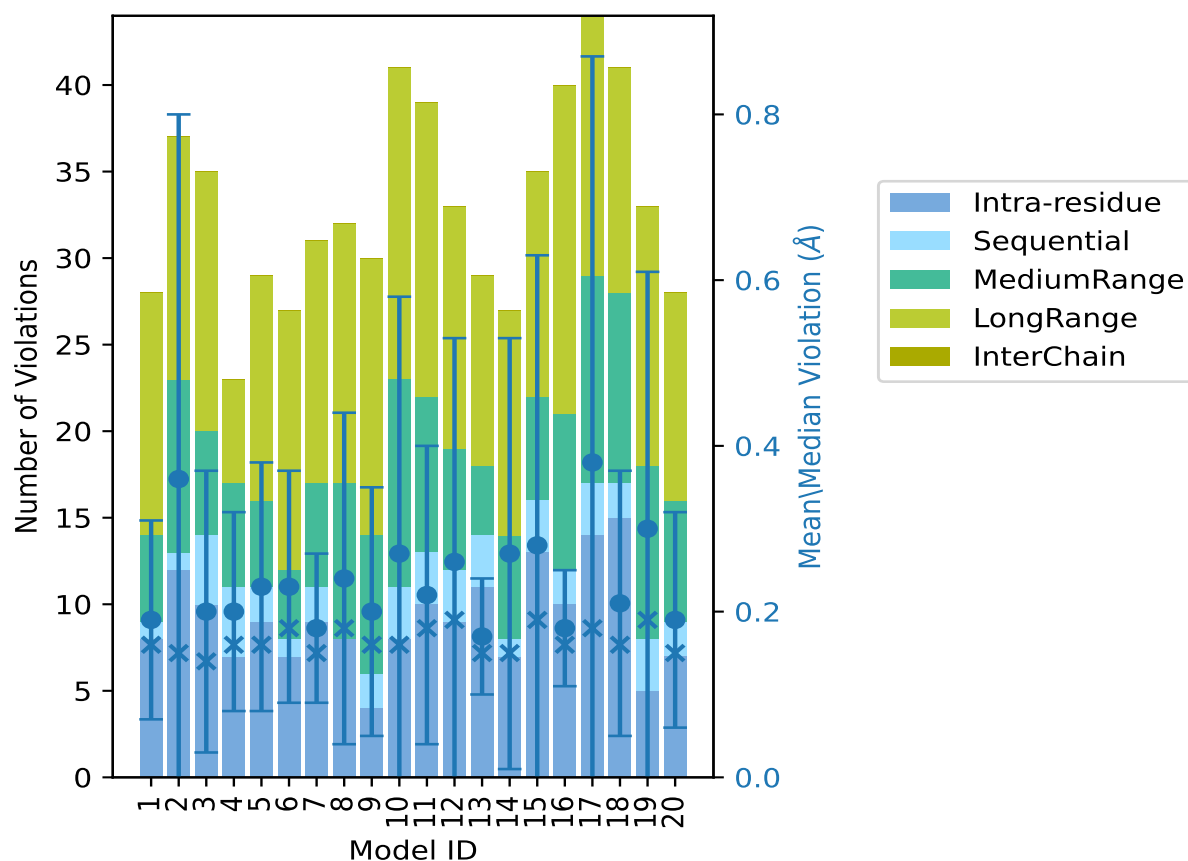
Continued from previous page...

| 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       | 10                   | 3               | 9               | 17              | 0               | 39    | 0.22     | 1.17    | 0.18                | 0.18       |
| 12       | 9                    | 3               | 7               | 14              | 0               | 33    | 0.26     | 1.65    | 0.27                | 0.19       |
| 13       | 11                   | 3               | 4               | 11              | 0               | 29    | 0.17     | 0.46    | 0.07                | 0.15       |
| 14       | 7                    | 1               | 6               | 13              | 0               | 27    | 0.27     | 1.08    | 0.26                | 0.15       |
| 15       | 13                   | 3               | 6               | 13              | 0               | 35    | 0.28     | 1.88    | 0.35                | 0.19       |
| 16       | 10                   | 2               | 9               | 19              | 0               | 40    | 0.18     | 0.38    | 0.07                | 0.16       |
| 17       | 14                   | 3               | 12              | 15              | 0               | 44    | 0.38     | 1.93    | 0.49                | 0.18       |
| 18       | 15                   | 2               | 11              | 13              | 0               | 41    | 0.21     | 0.98    | 0.16                | 0.16       |
| 19       | 5                    | 3               | 10              | 15              | 0               | 33    | 0.3      | 1.34    | 0.31                | 0.19       |
| 20       | 7                    | 2               | 7               | 12              | 0               | 28    | 0.19     | 0.78    | 0.13                | 0.15       |

<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

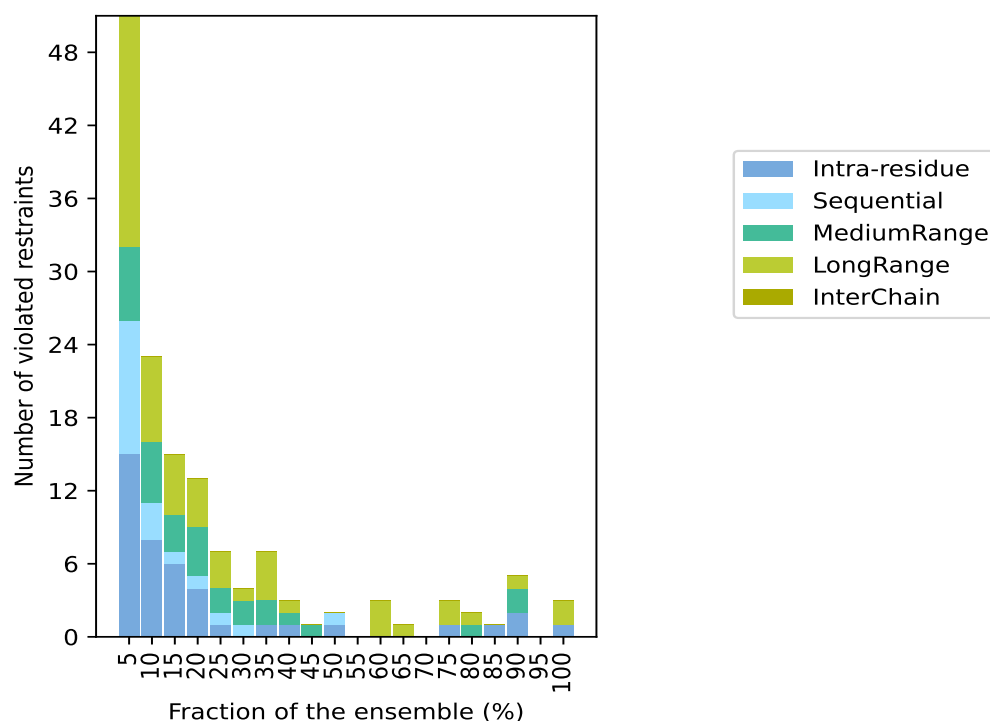
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 951(IR:261, SQ:232, MR:165, LR:293, IC:0) restraints are 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>       | %     |
| 15                            | 11              | 6               | 19              | 0               | 51    | 1                        | 5.0   |
| 8                             | 3               | 5               | 7               | 0               | 23    | 2                        | 10.0  |
| 6                             | 1               | 3               | 5               | 0               | 15    | 3                        | 15.0  |
| 4                             | 1               | 4               | 4               | 0               | 13    | 4                        | 20.0  |
| 1                             | 1               | 2               | 3               | 0               | 7     | 5                        | 25.0  |
| 0                             | 1               | 2               | 1               | 0               | 4     | 6                        | 30.0  |
| 1                             | 0               | 2               | 4               | 0               | 7     | 7                        | 35.0  |
| 1                             | 0               | 1               | 1               | 0               | 3     | 8                        | 40.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 9                        | 45.0  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 10                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 55.0  |
| 0                             | 0               | 0               | 3               | 0               | 3     | 12                       | 60.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 13                       | 65.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 14                       | 70.0  |
| 1                             | 0               | 0               | 2               | 0               | 3     | 15                       | 75.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 16                       | 80.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 17                       | 85.0  |
| 2                             | 0               | 2               | 1               | 0               | 5     | 18                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 95.0  |
| 1                             | 0               | 0               | 2               | 0               | 3     | 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](#)

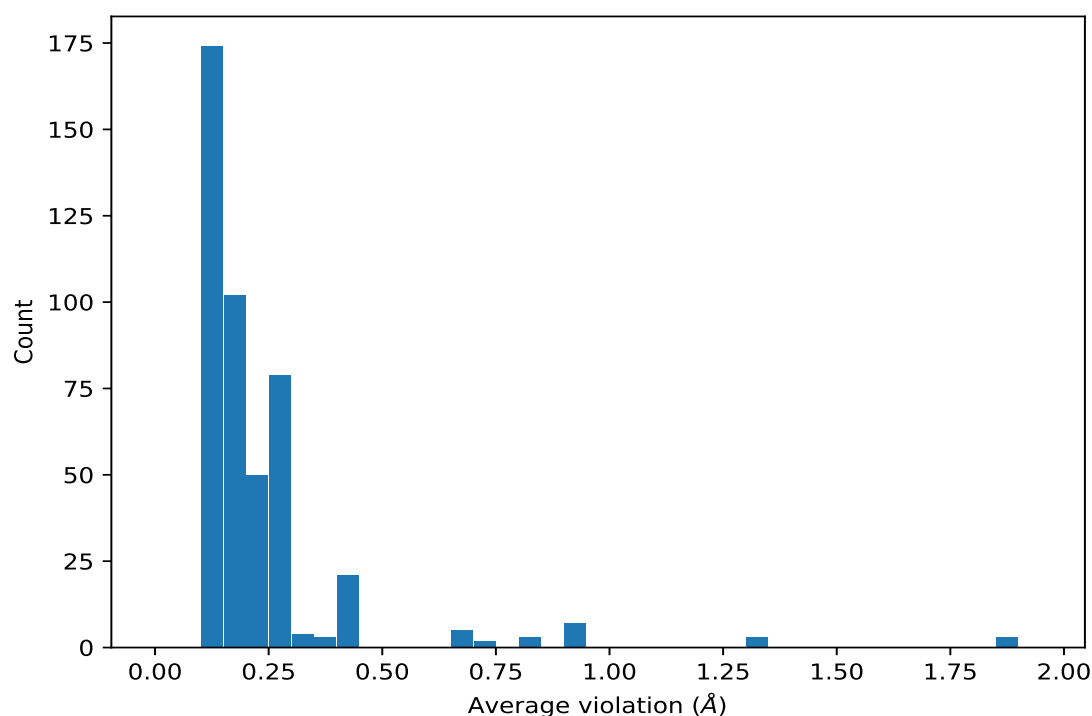


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 20                  | 0.33     | 0.1                 | 0.34       |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 20                  | 0.33     | 0.1                 | 0.34       |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 20                  | 0.33     | 0.1                 | 0.34       |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 20                  | 0.22     | 0.04                | 0.21       |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 20                  | 0.18     | 0.02                | 0.18       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 20                  | 0.18     | 0.02                | 0.18       |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 18                  | 0.7      | 0.31                | 0.67       |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 18                  | 0.4      | 0.13                | 0.4        |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 18                  | 0.4      | 0.13                | 0.4        |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 18                  | 0.4      | 0.13                | 0.4        |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 18                  | 0.18     | 0.11                | 0.15       |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 18                  | 0.18     | 0.11                | 0.15       |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 18                  | 0.18     | 0.11                | 0.15       |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 18                  | 0.18     | 0.11                | 0.15       |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 18                  | 0.18     | 0.11                | 0.15       |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 18                  | 0.18     | 0.11                | 0.15       |
| (1,714)  | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,714)  | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,714)  | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,714)  | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,714)  | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,714)  | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,714)  | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,714)  | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,714)  | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 18                  | 0.17     | 0.04                | 0.16       |
| (1,818)  | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 18                  | 0.13     | 0.01                | 0.13       |
| (1,818)  | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 18                  | 0.13     | 0.01                | 0.13       |
| (1,818)  | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 18                  | 0.13     | 0.01                | 0.13       |
| (1,818)  | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 18                  | 0.13     | 0.01                | 0.13       |
| (1,818)  | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 18                  | 0.13     | 0.01                | 0.13       |
| (1,818)  | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 18                  | 0.13     | 0.01                | 0.13       |
| (1,343)  | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 17                  | 0.12     | 0.02                | 0.12       |
| (1,343)  | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 17                  | 0.12     | 0.02                | 0.12       |
| (1,343)  | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 17                  | 0.12     | 0.02                | 0.12       |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 16                  | 0.2      | 0.06                | 0.18       |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 16                  | 0.2      | 0.06                | 0.18       |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 16                  | 0.2      | 0.06                | 0.18       |
| (1,263)  | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 16                  | 0.14     | 0.03                | 0.13       |
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 16                  | 0.14     | 0.03                | 0.13       |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 16                  | 0.14     | 0.03                | 0.13       |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 15                  | 0.28     | 0.13                | 0.23       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 15                  | 0.28     | 0.13                | 0.23       |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 15                  | 0.2      | 0.02                | 0.21       |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 15                  | 0.2      | 0.02                | 0.21       |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 15                  | 0.2      | 0.02                | 0.21       |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 15                  | 0.2      | 0.02                | 0.21       |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 15                  | 0.2      | 0.02                | 0.21       |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 15                  | 0.2      | 0.02                | 0.21       |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 15                  | 0.17     | 0.04                | 0.17       |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 15                  | 0.17     | 0.04                | 0.17       |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 15                  | 0.17     | 0.04                | 0.17       |
| (1,329) | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 13                  | 0.17     | 0.05                | 0.17       |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG11 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG12 | 12                  | 0.27     | 0.06                | 0.3        |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG13 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG21 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG22 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG23 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG11 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG12 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG13 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG21 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG22 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG23 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG11 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG12 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG13 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG21 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG22 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG23 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG11 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG12 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG13 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG21 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG22 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG23 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG11 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG12 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG13 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG21 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG22 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG23 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG11 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG12 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG13 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG21 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG22 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG23 | 12                  | 0.27     | 0.06                | 0.3        |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 12                  | 0.16     | 0.05                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,900)  | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,900)  | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 12                  | 0.16     | 0.05                | 0.15       |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 12                  | 0.14     | 0.03                | 0.12       |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 12                  | 0.14     | 0.03                | 0.12       |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 12                  | 0.14     | 0.03                | 0.12       |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 12                  | 0.14     | 0.03                | 0.12       |
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 10                  | 0.18     | 0.02                | 0.18       |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 10                  | 0.14     | 0.02                | 0.15       |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 10                  | 0.14     | 0.02                | 0.15       |
| (1,67)   | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 9                   | 0.19     | 0.05                | 0.19       |
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 9                   | 0.19     | 0.05                | 0.19       |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 9                   | 0.19     | 0.05                | 0.19       |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE2  | 8                   | 0.22     | 0.05                | 0.21       |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE3  | 8                   | 0.22     | 0.05                | 0.21       |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE2  | 8                   | 0.22     | 0.05                | 0.21       |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE3  | 8                   | 0.22     | 0.05                | 0.21       |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 8                   | 0.21     | 0.06                | 0.21       |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 8                   | 0.21     | 0.06                | 0.21       |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 8                   | 0.21     | 0.06                | 0.21       |
| (1,255)  | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 8                   | 0.15     | 0.02                | 0.15       |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 7                   | 0.94     | 0.54                | 0.96       |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 7                   | 0.94     | 0.54                | 0.96       |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 7                   | 0.94     | 0.54                | 0.96       |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 7                   | 0.94     | 0.54                | 0.96       |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 7                   | 0.94     | 0.54                | 0.96       |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 7                   | 0.94     | 0.54                | 0.96       |
| (1,576)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 7                   | 0.68     | 0.52                | 0.4        |
| (1,576)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 7                   | 0.68     | 0.52                | 0.4        |
| (1,576)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 7                   | 0.68     | 0.52                | 0.4        |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD11 | 7                   | 0.36     | 0.13                | 0.39       |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD12 | 7                   | 0.36     | 0.13                | 0.39       |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD13 | 7                   | 0.36     | 0.13                | 0.39       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,876)  | 1:17:A:VAL:HG11 | 1:57:A:ASN:HD21 | 7                   | 0.27     | 0.07                | 0.25       |
| (1,876)  | 1:17:A:VAL:HG12 | 1:57:A:ASN:HD21 | 7                   | 0.27     | 0.07                | 0.25       |
| (1,876)  | 1:17:A:VAL:HG13 | 1:57:A:ASN:HD21 | 7                   | 0.27     | 0.07                | 0.25       |
| (1,876)  | 1:17:A:VAL:HG21 | 1:57:A:ASN:HD21 | 7                   | 0.27     | 0.07                | 0.25       |
| (1,876)  | 1:17:A:VAL:HG22 | 1:57:A:ASN:HD21 | 7                   | 0.27     | 0.07                | 0.25       |
| (1,876)  | 1:17:A:VAL:HG23 | 1:57:A:ASN:HD21 | 7                   | 0.27     | 0.07                | 0.25       |
| (1,631)  | 1:10:A:LEU:HA   | 1:10:A:LEU:HD21 | 7                   | 0.18     | 0.02                | 0.19       |
| (1,631)  | 1:10:A:LEU:HA   | 1:10:A:LEU:HD22 | 7                   | 0.18     | 0.02                | 0.19       |
| (1,631)  | 1:10:A:LEU:HA   | 1:10:A:LEU:HD23 | 7                   | 0.18     | 0.02                | 0.19       |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD11 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD12 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD13 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD21 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD22 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD23 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD11 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD12 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD13 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD21 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD22 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD23 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD11 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD12 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD13 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD21 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD22 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD23 | 7                   | 0.14     | 0.02                | 0.13       |
| (1,705)  | 1:42:A:THR:HG21 | 1:58:A:PRO:HG3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,705)  | 1:42:A:THR:HG22 | 1:58:A:PRO:HG3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,705)  | 1:42:A:THR:HG23 | 1:58:A:PRO:HG3  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD11 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD12 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD13 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD21 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD22 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD23 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD11 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD12 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD13 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD21 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD22 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD23 | 6                   | 0.4      | 0.2                 | 0.36       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD11 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD12 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD13 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD21 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD22 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD23 | 6                   | 0.4      | 0.2                 | 0.36       |
| (1,814)  | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG2   | 6                   | 0.2      | 0.03                | 0.2        |
| (1,814)  | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG3   | 6                   | 0.2      | 0.03                | 0.2        |
| (1,814)  | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG2   | 6                   | 0.2      | 0.03                | 0.2        |
| (1,814)  | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG3   | 6                   | 0.2      | 0.03                | 0.2        |
| (1,814)  | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG2   | 6                   | 0.2      | 0.03                | 0.2        |
| (1,814)  | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG3   | 6                   | 0.2      | 0.03                | 0.2        |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG11 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG12 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG13 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG21 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG22 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG23 | 6                   | 0.12     | 0.02                | 0.12       |
| (1,969)  | 1:39:A:CYS:HA   | 1:40:A:PRO:HD2  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,969)  | 1:39:A:CYS:HA   | 1:40:A:PRO:HD3  | 6                   | 0.11     | 0.01                | 0.11       |
| (1,571)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 5                   | 1.34     | 0.31                | 1.25       |
| (1,571)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 5                   | 1.34     | 0.31                | 1.25       |
| (1,571)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 5                   | 1.34     | 0.31                | 1.25       |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE21 | 5                   | 0.23     | 0.04                | 0.22       |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE22 | 5                   | 0.23     | 0.04                | 0.22       |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE21 | 5                   | 0.23     | 0.04                | 0.22       |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE22 | 5                   | 0.23     | 0.04                | 0.22       |
| (1,586)  | 1:27:A:ILE:HD11 | 1:62:A:TRP:HZ3  | 5                   | 0.15     | 0.05                | 0.13       |
| (1,586)  | 1:27:A:ILE:HD12 | 1:62:A:TRP:HZ3  | 5                   | 0.15     | 0.05                | 0.13       |
| (1,586)  | 1:27:A:ILE:HD13 | 1:62:A:TRP:HZ3  | 5                   | 0.15     | 0.05                | 0.13       |
| (1,1082) | 1:70:A:VAL:HG11 | 1:71:A:GLN:H    | 5                   | 0.15     | 0.04                | 0.14       |
| (1,1082) | 1:70:A:VAL:HG12 | 1:71:A:GLN:H    | 5                   | 0.15     | 0.04                | 0.14       |
| (1,1082) | 1:70:A:VAL:HG13 | 1:71:A:GLN:H    | 5                   | 0.15     | 0.04                | 0.14       |
| (1,1082) | 1:70:A:VAL:HG21 | 1:71:A:GLN:H    | 5                   | 0.15     | 0.04                | 0.14       |
| (1,1082) | 1:70:A:VAL:HG22 | 1:71:A:GLN:H    | 5                   | 0.15     | 0.04                | 0.14       |
| (1,1082) | 1:70:A:VAL:HG23 | 1:71:A:GLN:H    | 5                   | 0.15     | 0.04                | 0.14       |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD11 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD12 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD13 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD21 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD22 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD23 | 5                   | 0.14     | 0.02                | 0.15       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,812)  | 1:1:A:MET:HE2   | 1:66:A:LEU:HD11 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE2   | 1:66:A:LEU:HD12 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE2   | 1:66:A:LEU:HD13 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE2   | 1:66:A:LEU:HD21 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE2   | 1:66:A:LEU:HD22 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE2   | 1:66:A:LEU:HD23 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE3   | 1:66:A:LEU:HD11 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE3   | 1:66:A:LEU:HD12 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE3   | 1:66:A:LEU:HD13 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE3   | 1:66:A:LEU:HD21 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE3   | 1:66:A:LEU:HD22 | 5                   | 0.14     | 0.02                | 0.15       |
| (1,812)  | 1:1:A:MET:HE3   | 1:66:A:LEU:HD23 | 5                   | 0.14     | 0.02                | 0.15       |
| (3,19)   | 1:33:A:THR:O    | 1:43:A:GLU:H    | 5                   | 0.13     | 0.03                | 0.12       |
| (1,297)  | 1:58:A:PRO:HA   | 1:63:A:LEU:HD21 | 5                   | 0.12     | 0.02                | 0.12       |
| (1,297)  | 1:58:A:PRO:HA   | 1:63:A:LEU:HD22 | 5                   | 0.12     | 0.02                | 0.12       |
| (1,297)  | 1:58:A:PRO:HA   | 1:63:A:LEU:HD23 | 5                   | 0.12     | 0.02                | 0.12       |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB2  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB3  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB2  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB3  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB2  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB3  | 5                   | 0.11     | 0.01                | 0.11       |
| (1,472)  | 1:63:A:LEU:HD21 | 1:64:A:GLN:HE21 | 4                   | 1.86     | 0.15                | 1.84       |
| (1,472)  | 1:63:A:LEU:HD22 | 1:64:A:GLN:HE21 | 4                   | 1.86     | 0.15                | 1.84       |
| (1,472)  | 1:63:A:LEU:HD23 | 1:64:A:GLN:HE21 | 4                   | 1.86     | 0.15                | 1.84       |
| (1,471)  | 1:64:A:GLN:HE21 | 1:67:A:LEU:HG   | 4                   | 0.91     | 0.23                | 0.91       |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD11 | 4                   | 0.84     | 0.36                | 0.86       |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD12 | 4                   | 0.84     | 0.36                | 0.86       |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD13 | 4                   | 0.84     | 0.36                | 0.86       |
| (1,644)  | 1:26:A:ILE:HA   | 1:49:A:LYS:HB2  | 4                   | 0.7      | 0.32                | 0.82       |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG2  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 4                   | 0.2      | 0.03                | 0.2        |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG11 | 4                   | 0.17     | 0.05                | 0.16       |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG12 | 4                   | 0.17     | 0.05                | 0.16       |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG13 | 4                   | 0.17     | 0.05                | 0.16       |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 4                   | 0.17     | 0.05                | 0.16       |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 4                   | 0.17     | 0.05                | 0.16       |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 4                   | 0.17     | 0.05                | 0.16       |
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG11 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG12 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG13 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG11 | 4                   | 0.16     | 0.02                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG12 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG13 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG11 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG12 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG13 | 4                   | 0.16     | 0.02                | 0.16       |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD11 | 4                   | 0.14     | 0.01                | 0.14       |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD12 | 4                   | 0.14     | 0.01                | 0.14       |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD13 | 4                   | 0.14     | 0.01                | 0.14       |
| (1,875)  | 1:17:A:VAL:HG11 | 1:57:A:ASN:HB3  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,875)  | 1:17:A:VAL:HG12 | 1:57:A:ASN:HB3  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,875)  | 1:17:A:VAL:HG13 | 1:57:A:ASN:HB3  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,875)  | 1:17:A:VAL:HG21 | 1:57:A:ASN:HB3  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,875)  | 1:17:A:VAL:HG22 | 1:57:A:ASN:HB3  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,875)  | 1:17:A:VAL:HG23 | 1:57:A:ASN:HB3  | 4                   | 0.14     | 0.01                | 0.14       |
| (1,771)  | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG21 | 4                   | 0.14     | 0.03                | 0.12       |
| (1,771)  | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG22 | 4                   | 0.14     | 0.03                | 0.12       |
| (1,771)  | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG23 | 4                   | 0.14     | 0.03                | 0.12       |
| (1,1077) | 1:68:A:ARG:HA   | 1:71:A:GLN:HE21 | 4                   | 0.14     | 0.01                | 0.14       |
| (1,1077) | 1:68:A:ARG:HA   | 1:71:A:GLN:HE22 | 4                   | 0.14     | 0.01                | 0.14       |
| (1,205)  | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,252)  | 1:57:A:ASN:HB2  | 1:57:A:ASN:HD22 | 4                   | 0.12     | 0.02                | 0.11       |
| (3,27)   | 1:48:A:THR:H    | 1:52:A:LYS:O    | 4                   | 0.12     | 0.01                | 0.12       |
| (1,449)  | 1:10:A:LEU:H    | 1:10:A:LEU:HD21 | 3                   | 0.23     | 0.04                | 0.21       |
| (1,449)  | 1:10:A:LEU:H    | 1:10:A:LEU:HD22 | 3                   | 0.23     | 0.04                | 0.21       |
| (1,449)  | 1:10:A:LEU:H    | 1:10:A:LEU:HD23 | 3                   | 0.23     | 0.04                | 0.21       |
| (1,1075) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD2  | 3                   | 0.22     | 0.02                | 0.23       |
| (1,1075) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD3  | 3                   | 0.22     | 0.02                | 0.23       |
| (1,884)  | 1:21:A:VAL:HG11 | 1:62:A:TRP:HB2  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG11 | 1:62:A:TRP:HB3  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG12 | 1:62:A:TRP:HB2  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG12 | 1:62:A:TRP:HB3  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG13 | 1:62:A:TRP:HB2  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG13 | 1:62:A:TRP:HB3  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG21 | 1:62:A:TRP:HB2  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG21 | 1:62:A:TRP:HB3  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG22 | 1:62:A:TRP:HB2  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG22 | 1:62:A:TRP:HB3  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG23 | 1:62:A:TRP:HB2  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,884)  | 1:21:A:VAL:HG23 | 1:62:A:TRP:HB3  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,673)  | 1:42:A:THR:HB   | 1:58:A:PRO:HG3  | 3                   | 0.17     | 0.02                | 0.17       |
| (1,604)  | 1:22:A:VAL:HB   | 1:62:A:TRP:HH2  | 3                   | 0.16     | 0.01                | 0.16       |
| (1,453)  | 1:11:A:LYS:H    | 1:11:A:LYS:HG2  | 3                   | 0.16     | 0.01                | 0.16       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,285)  | 1:44:A:VAL:HG21 | 1:58:A:PRO:HB3  | 3                   | 0.15     | 0.01                | 0.14       |
| (1,285)  | 1:44:A:VAL:HG22 | 1:58:A:PRO:HB3  | 3                   | 0.15     | 0.01                | 0.14       |
| (1,285)  | 1:44:A:VAL:HG23 | 1:58:A:PRO:HB3  | 3                   | 0.15     | 0.01                | 0.14       |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD21 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD22 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD23 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,645)  | 1:61:A:LYS:HA   | 1:61:A:LYS:HD2  | 3                   | 0.14     | 0.03                | 0.15       |
| (1,2)    | 1:13:A:ARG:H    | 1:14:A:CYS:H    | 3                   | 0.13     | 0.02                | 0.14       |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD11 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD12 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD13 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD21 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD22 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD23 | 3                   | 0.13     | 0.01                | 0.13       |
| (1,289)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD11 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,289)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD12 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,289)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD13 | 3                   | 0.13     | 0.02                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD21 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD22 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD23 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD21 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD22 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD23 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD21 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD22 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,699)  | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD23 | 3                   | 0.13     | 0.03                | 0.12       |
| (1,66)   | 1:18:A:ILE:HG21 | 1:20:A:THR:H    | 3                   | 0.12     | 0.01                | 0.11       |
| (1,66)   | 1:18:A:ILE:HG22 | 1:20:A:THR:H    | 3                   | 0.12     | 0.01                | 0.11       |
| (1,66)   | 1:18:A:ILE:HG23 | 1:20:A:THR:H    | 3                   | 0.12     | 0.01                | 0.11       |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG11 | 3                   | 0.12     | 0.01                | 0.12       |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG12 | 3                   | 0.12     | 0.01                | 0.12       |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG13 | 3                   | 0.12     | 0.01                | 0.12       |
| (1,813)  | 1:2:A:ILE:HB    | 1:29:A:ARG:HD2  | 2                   | 0.68     | 0.11                | 0.68       |
| (1,813)  | 1:2:A:ILE:HB    | 1:29:A:ARG:HD3  | 2                   | 0.68     | 0.11                | 0.68       |
| (1,658)  | 1:68:A:ARG:HA   | 1:68:A:ARG:HD3  | 2                   | 0.32     | 0.02                | 0.32       |
| (1,254)  | 1:57:A:ASN:HD22 | 1:60:A:ALA:HA   | 2                   | 0.27     | 0.11                | 0.27       |
| (1,426)  | 1:10:A:LEU:H    | 1:11:A:LYS:H    | 2                   | 0.21     | 0.05                | 0.21       |
| (1,445)  | 1:4:A:GLU:H     | 1:4:A:GLU:HG2   | 2                   | 0.2      | 0.01                | 0.2        |
| (1,948)  | 1:30:A:ILE:HD11 | 1:66:A:LEU:HB2  | 2                   | 0.2      | 0.02                | 0.2        |
| (1,948)  | 1:30:A:ILE:HD11 | 1:66:A:LEU:HB3  | 2                   | 0.2      | 0.02                | 0.2        |
| (1,948)  | 1:30:A:ILE:HD12 | 1:66:A:LEU:HB2  | 2                   | 0.2      | 0.02                | 0.2        |
| (1,948)  | 1:30:A:ILE:HD12 | 1:66:A:LEU:HB3  | 2                   | 0.2      | 0.02                | 0.2        |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,948) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HB2  | 2                   | 0.2      | 0.02                | 0.2        |
| (1,948) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HB3  | 2                   | 0.2      | 0.02                | 0.2        |
| (1,867) | 1:17:A:VAL:HG11 | 1:55:A:CYS:CB   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,867) | 1:17:A:VAL:HG12 | 1:55:A:CYS:CB   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,867) | 1:17:A:VAL:HG13 | 1:55:A:CYS:CB   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,867) | 1:17:A:VAL:HG21 | 1:55:A:CYS:CB   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,867) | 1:17:A:VAL:HG22 | 1:55:A:CYS:CB   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,867) | 1:17:A:VAL:HG23 | 1:55:A:CYS:CB   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,459) | 1:13:A:ARG:H    | 1:13:A:ARG:HG2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,619) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD21 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,619) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD22 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,619) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD23 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG21  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG22  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG23  | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD11 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD12 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD13 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,256) | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB3  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD21 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD22 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD23 | 2                   | 0.12     | 0.01                | 0.12       |
| (1,870) | 1:17:A:VAL:HG11 | 1:57:A:ASN:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,870) | 1:17:A:VAL:HG12 | 1:57:A:ASN:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,870) | 1:17:A:VAL:HG13 | 1:57:A:ASN:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,870) | 1:17:A:VAL:HG21 | 1:57:A:ASN:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,870) | 1:17:A:VAL:HG22 | 1:57:A:ASN:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,870) | 1:17:A:VAL:HG23 | 1:57:A:ASN:H    | 2                   | 0.12     | 0.02                | 0.12       |
| (1,924) | 1:27:A:ILE:HG21 | 1:30:A:ILE:HG12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,924) | 1:27:A:ILE:HG21 | 1:30:A:ILE:HG13 | 2                   | 0.12     | 0.02                | 0.12       |

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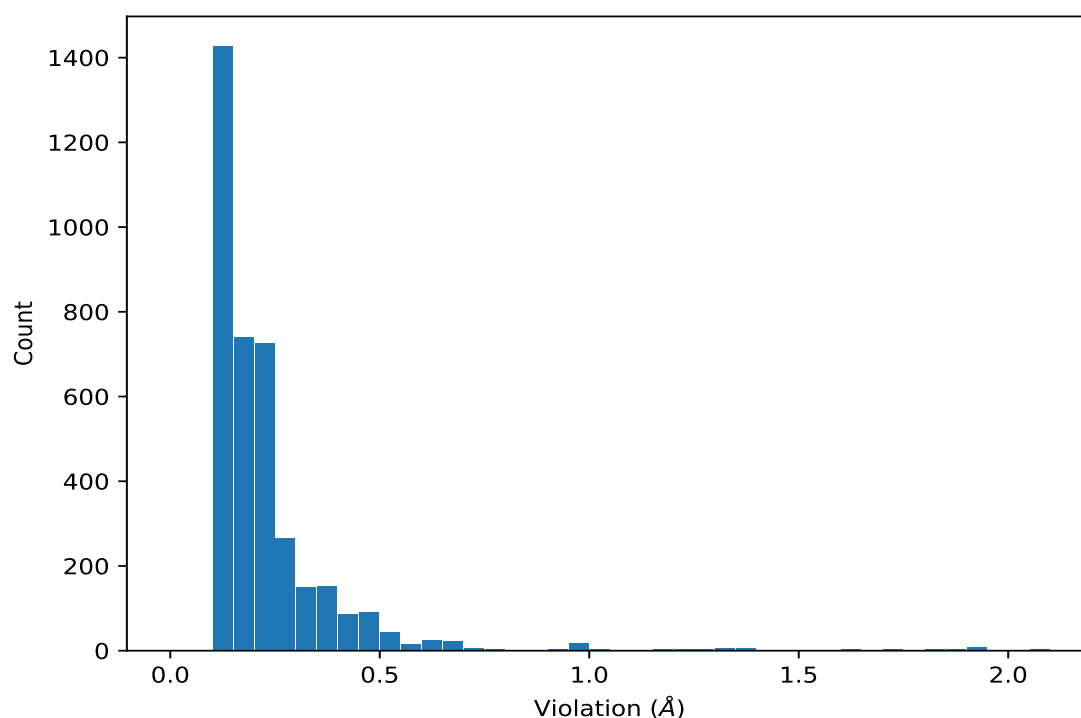
| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,924) | 1:27:A:ILE:HG22 | 1:30:A:ILE:HG12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,924) | 1:27:A:ILE:HG22 | 1:30:A:ILE:HG13 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,924) | 1:27:A:ILE:HG23 | 1:30:A:ILE:HG12 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,924) | 1:27:A:ILE:HG23 | 1:30:A:ILE:HG13 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,147) | 1:49:A:LYS:H    | 1:49:A:LYS:HG2  | 2                   | 0.12     | 0.02                | 0.12       |
| (1,215) | 1:66:A:LEU:H    | 1:66:A:LEU:HD11 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,215) | 1:66:A:LEU:H    | 1:66:A:LEU:HD12 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,215) | 1:66:A:LEU:H    | 1:66:A:LEU:HD13 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD23 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,846) | 1:10:A:LEU:HB2  | 1:11:A:LYS:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,846) | 1:10:A:LEU:HB3  | 1:11:A:LYS:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (3,15)  | 1:4:A:GLU:O     | 1:32:A:VAL:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,646) | 1:61:A:LYS:HA   | 1:61:A:LYS:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,661) | 1:66:A:LEU:HA   | 1:69:A:HIS:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,921) | 1:26:A:ILE:HA   | 1:49:A:LYS:HG2  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,921) | 1:26:A:ILE:HA   | 1:49:A:LYS:HG3  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,649) | 1:78:A:THR:HA   | 1:79:A:PRO:HD3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (3,35)  | 1:64:A:GLN:O    | 1:68:A:ARG:H    | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,472)  | 1:63:A:LEU:HD21 | 1:64:A:GLN:HE21 | 2        | 2.08          |
| (1,472)  | 1:63:A:LEU:HD22 | 1:64:A:GLN:HE21 | 2        | 2.08          |
| (1,472)  | 1:63:A:LEU:HD23 | 1:64:A:GLN:HE21 | 2        | 2.08          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 17       | 1.93          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 17       | 1.93          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 17       | 1.93          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 17       | 1.93          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 17       | 1.93          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 17       | 1.93          |
| (1,571)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 17       | 1.93          |
| (1,571)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 17       | 1.93          |
| (1,571)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 17       | 1.93          |
| (1,472)  | 1:63:A:LEU:HD21 | 1:64:A:GLN:HE21 | 15       | 1.88          |
| (1,472)  | 1:63:A:LEU:HD22 | 1:64:A:GLN:HE21 | 15       | 1.88          |
| (1,472)  | 1:63:A:LEU:HD23 | 1:64:A:GLN:HE21 | 15       | 1.88          |
| (1,472)  | 1:63:A:LEU:HD21 | 1:64:A:GLN:HE21 | 17       | 1.81          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,472)  | 1:63:A:LEU:HD22 | 1:64:A:GLN:HE21 | 17       | 1.81          |
| (1,472)  | 1:63:A:LEU:HD23 | 1:64:A:GLN:HE21 | 17       | 1.81          |
| (1,576)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 17       | 1.72          |
| (1,576)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 17       | 1.72          |
| (1,576)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 17       | 1.72          |
| (1,472)  | 1:63:A:LEU:HD21 | 1:64:A:GLN:HE21 | 12       | 1.65          |
| (1,472)  | 1:63:A:LEU:HD22 | 1:64:A:GLN:HE21 | 12       | 1.65          |
| (1,472)  | 1:63:A:LEU:HD23 | 1:64:A:GLN:HE21 | 12       | 1.65          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 10       | 1.39          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 10       | 1.39          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 10       | 1.39          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 10       | 1.39          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 10       | 1.39          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 10       | 1.39          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 19       | 1.34          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD11 | 2        | 1.32          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD12 | 2        | 1.32          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD13 | 2        | 1.32          |
| (1,571)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 19       | 1.31          |
| (1,571)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 19       | 1.31          |
| (1,571)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 19       | 1.31          |
| (1,571)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 2        | 1.25          |
| (1,571)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 2        | 1.25          |
| (1,571)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 2        | 1.25          |
| (1,576)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 10       | 1.24          |
| (1,576)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 10       | 1.24          |
| (1,576)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 10       | 1.24          |
| (1,471)  | 1:64:A:GLN:HE21 | 1:67:A:LEU:HG   | 2        | 1.21          |
| (1,571)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 10       | 1.2           |
| (1,571)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 10       | 1.2           |
| (1,571)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 10       | 1.2           |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 11       | 1.17          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 14       | 1.08          |
| (1,471)  | 1:64:A:GLN:HE21 | 1:67:A:LEU:HG   | 15       | 1.04          |
| (1,571)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 14       | 1.02          |
| (1,571)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 14       | 1.02          |
| (1,571)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 14       | 1.02          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 19       | 0.99          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 19       | 0.99          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 19       | 0.99          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 19       | 0.99          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 19       | 0.99          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 19       | 0.99          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD11 | 15       | 0.99          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD12 | 15       | 0.99          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD13 | 15       | 0.99          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 18       | 0.98          |
| (1,644)  | 1:26:A:ILE:HA   | 1:49:A:LYS:HB2  | 8        | 0.97          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 2        | 0.96          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 2        | 0.96          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 2        | 0.96          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 2        | 0.96          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 2        | 0.96          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 2        | 0.96          |
| (1,644)  | 1:26:A:ILE:HA   | 1:49:A:LYS:HB2  | 3        | 0.94          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 8        | 0.94          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 9        | 0.94          |
| (1,813)  | 1:2:A:ILE:HB    | 1:29:A:ARG:HD2  | 17       | 0.79          |
| (1,813)  | 1:2:A:ILE:HB    | 1:29:A:ARG:HD3  | 17       | 0.79          |
| (1,471)  | 1:64:A:GLN:HE21 | 1:67:A:LEU:HG   | 17       | 0.78          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 20       | 0.78          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 2        | 0.74          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD11 | 17       | 0.72          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD12 | 17       | 0.72          |
| (1,91)   | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD13 | 17       | 0.72          |
| (1,644)  | 1:26:A:ILE:HA   | 1:49:A:LYS:HB2  | 10       | 0.71          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 1        | 0.69          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD11 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD12 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD13 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD21 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD22 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD23 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD11 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD12 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD13 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD21 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD22 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD23 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD11 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD12 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD13 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD21 | 3        | 0.68          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD22 | 3        | 0.68          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD23 | 3        | 0.68          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 2        | 0.66          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 2        | 0.66          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 2        | 0.66          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 6        | 0.65          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 4        | 0.64          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD11 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD12 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD13 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD21 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD22 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD23 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD11 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD12 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD13 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD21 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD22 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD23 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD11 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD12 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD13 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD21 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD22 | 5        | 0.62          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD23 | 5        | 0.62          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 5        | 0.62          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 5        | 0.62          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 5        | 0.62          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 5        | 0.62          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 5        | 0.62          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 5        | 0.62          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 14       | 0.6           |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 14       | 0.6           |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 14       | 0.6           |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 14       | 0.6           |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 14       | 0.6           |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 14       | 0.6           |
| (1,471)  | 1:64:A:GLN:HE21 | 1:67:A:LEU:HG   | 12       | 0.6           |
| (1,813)  | 1:2:A:ILE:HB    | 1:29:A:ARG:HD2  | 6        | 0.58          |
| (1,813)  | 1:2:A:ILE:HB    | 1:29:A:ARG:HD3  | 6        | 0.58          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 18       | 0.58          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 18       | 0.58          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 18       | 0.58          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD11 | 14       | 0.55          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD12 | 14       | 0.55          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD13 | 14       | 0.55          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 7        | 0.54          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 7        | 0.54          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 7        | 0.54          |
| (1,223) | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 5        | 0.53          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 12       | 0.51          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 12       | 0.51          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 12       | 0.51          |
| (1,223) | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 10       | 0.51          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 5        | 0.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 5        | 0.5           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 5        | 0.5           |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 15       | 0.48          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 15       | 0.48          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 15       | 0.48          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 19       | 0.47          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 19       | 0.47          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 19       | 0.47          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 11       | 0.46          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 11       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 14       | 0.46          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 14       | 0.46          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 13       | 0.46          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 13       | 0.46          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 13       | 0.46          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 5        | 0.46          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 5        | 0.46          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 5        | 0.46          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 1        | 0.45          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 1        | 0.45          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 1        | 0.45          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 14       | 0.45          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 14       | 0.45          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 14       | 0.45          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 4        | 0.44          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 4        | 0.44          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 4        | 0.44          |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD11 | 6        | 0.44          |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD12 | 6        | 0.44          |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD13 | 6        | 0.44          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 17       | 0.44          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 17       | 0.44          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 17       | 0.44          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 3        | 0.44          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD11 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD12 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD13 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD21 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD22 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD23 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD11 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD12 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD13 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD21 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD22 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD23 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD11 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD12 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD13 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD21 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD22 | 18       | 0.43          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD23 | 18       | 0.43          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 18       | 0.42          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 18       | 0.42          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 18       | 0.42          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 18       | 0.42          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 18       | 0.42          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 18       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 15       | 0.42          |
| (1,918)  | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 15       | 0.42          |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD11 | 19       | 0.42          |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD12 | 19       | 0.42          |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD13 | 19       | 0.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 7        | 0.41          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 7        | 0.41          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 7        | 0.41          |
| (1,576) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 19       | 0.41          |
| (1,576) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 19       | 0.41          |
| (1,576) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 19       | 0.41          |
| (1,223) | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 12       | 0.41          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 6        | 0.4           |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 6        | 0.4           |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 6        | 0.4           |
| (1,576) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 2        | 0.4           |
| (1,576) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 2        | 0.4           |
| (1,576) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 2        | 0.4           |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 14       | 0.39          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 14       | 0.39          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 14       | 0.39          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 17       | 0.39          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 17       | 0.39          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 17       | 0.39          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD11 | 12       | 0.39          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD12 | 12       | 0.39          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD13 | 12       | 0.39          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 1        | 0.39          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 1        | 0.39          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 1        | 0.39          |
| (1,223) | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 17       | 0.39          |
| (1,876) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HD21 | 6        | 0.38          |
| (1,876) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HD21 | 6        | 0.38          |
| (1,876) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HD21 | 6        | 0.38          |
| (1,876) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HD21 | 6        | 0.38          |
| (1,876) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HD21 | 6        | 0.38          |
| (1,876) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HD21 | 6        | 0.38          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 11       | 0.38          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 11       | 0.38          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 11       | 0.38          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 16       | 0.38          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 16       | 0.38          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 16       | 0.38          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 9        | 0.38          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 9        | 0.38          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 9        | 0.38          |
| (1,254) | 1:57:A:ASN:HD22 | 1:60:A:ALA:HA   | 17       | 0.38          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 9        | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 19       | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 19       | 0.37          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 19       | 0.37          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG11 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG12 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG13 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG21 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG22 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG23 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG11 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG12 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG13 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG21 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG22 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG23 | 2        | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG11 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG12 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG13 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG21 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG22 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG23 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG11 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG12 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG13 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG21 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG22 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG23 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG11 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG12 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG13 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG21 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG22 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG23 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG11 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG12 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG13 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG21 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG22 | 2        | 0.37          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG23 | 2        | 0.37          |
| (1,657) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD2  | 2        | 0.37          |
| (1,576) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 16       | 0.37          |
| (1,576) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 16       | 0.37          |
| (1,576) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 16       | 0.37          |
| (1,876) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HD21 | 3        | 0.36          |
| (1,876) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HD21 | 3        | 0.36          |
| (1,876) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HD21 | 3        | 0.36          |
| (1,876) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HD21 | 3        | 0.36          |
| (1,876) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HD21 | 3        | 0.36          |
| (1,876) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HD21 | 3        | 0.36          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 10       | 0.36          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 10       | 0.36          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 10       | 0.36          |
| (1,576) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 18       | 0.36          |
| (1,576) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 18       | 0.36          |
| (1,576) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 18       | 0.36          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 8        | 0.35          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 8        | 0.35          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 8        | 0.35          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD11 | 13       | 0.34          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD12 | 13       | 0.34          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD13 | 13       | 0.34          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 16       | 0.34          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 16       | 0.34          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 16       | 0.34          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 18       | 0.34          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 18       | 0.34          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 18       | 0.34          |
| (1,658) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD3  | 11       | 0.34          |
| (1,239) | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 8        | 0.34          |
| (1,239) | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 8        | 0.34          |
| (1,239) | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 8        | 0.34          |
| (1,91)  | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD11 | 12       | 0.34          |
| (1,91)  | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD12 | 12       | 0.34          |
| (1,91)  | 1:64:A:GLN:HE21 | 1:67:A:LEU:HD13 | 12       | 0.34          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 5        | 0.33          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 5        | 0.33          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 5        | 0.33          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 19       | 0.33          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 19       | 0.33          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 19       | 0.33          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG11 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG12 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG13 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG21 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG22 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG23 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG11 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG12 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG13 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG21 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG22 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG23 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG11 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG12 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG13 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG21 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG22 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG23 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG11 | 10       | 0.32          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG12 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG13 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG21 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG22 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG23 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG11 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG12 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG13 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG21 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG22 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG23 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG11 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG12 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG13 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG21 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG22 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG23 | 10       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG11 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG12 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG13 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG21 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG22 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG23 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG11 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG12 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG13 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG21 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG22 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG23 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG11 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG12 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG13 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG21 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG22 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG23 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG11 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG12 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG13 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG21 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG22 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG23 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG11 | 20       | 0.32          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG12 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG13 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG21 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG22 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG23 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG11 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG12 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG13 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG21 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG22 | 20       | 0.32          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG23 | 20       | 0.32          |
| (1,803) | 1:22:A:VAL:CG2 | 1:26:A:ILE:HG21 | 8        | 0.32          |
| (1,803) | 1:22:A:VAL:CG2 | 1:26:A:ILE:HG22 | 8        | 0.32          |
| (1,803) | 1:22:A:VAL:CG2 | 1:26:A:ILE:HG23 | 8        | 0.32          |
| (1,681) | 1:44:A:VAL:HB  | 1:56:A:VAL:HG21 | 2        | 0.32          |
| (1,681) | 1:44:A:VAL:HB  | 1:56:A:VAL:HG22 | 2        | 0.32          |
| (1,681) | 1:44:A:VAL:HB  | 1:56:A:VAL:HG23 | 2        | 0.32          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG11 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG12 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG13 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG21 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG22 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG23 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG11 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG12 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG13 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG21 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG22 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG23 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG11 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG12 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG13 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG21 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG22 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG23 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG11 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG12 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG13 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG21 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG22 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG23 | 8        | 0.31          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG11 | 8        | 0.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,825)  | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG12 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG13 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG21 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG22 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG23 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG11 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG12 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG13 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG21 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG22 | 8        | 0.31          |
| (1,825)  | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG23 | 8        | 0.31          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 15       | 0.31          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 15       | 0.31          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 15       | 0.31          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 15       | 0.31          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 15       | 0.31          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 15       | 0.31          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 15       | 0.31          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 15       | 0.31          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 15       | 0.31          |
| (1,658)  | 1:68:A:ARG:HA   | 1:68:A:ARG:HD3  | 18       | 0.31          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD11 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD12 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD13 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD21 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD22 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD23 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD11 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD12 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD13 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD21 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD22 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD23 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD11 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD12 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD13 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD21 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD22 | 17       | 0.3           |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD23 | 17       | 0.3           |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE2  | 4        | 0.3           |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE3  | 4        | 0.3           |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE2  | 4        | 0.3           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,974) | 1:41:A:LYS:HB3 | 1:41:A:LYS:HE3  | 4        | 0.3           |
| (1,974) | 1:41:A:LYS:HB2 | 1:41:A:LYS:HE2  | 7        | 0.3           |
| (1,974) | 1:41:A:LYS:HB2 | 1:41:A:LYS:HE3  | 7        | 0.3           |
| (1,974) | 1:41:A:LYS:HB3 | 1:41:A:LYS:HE2  | 7        | 0.3           |
| (1,974) | 1:41:A:LYS:HB3 | 1:41:A:LYS:HE3  | 7        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG11 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG12 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG13 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG21 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG22 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG23 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG11 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG12 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG13 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG21 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG22 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG23 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG11 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG12 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG13 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG21 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG22 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG23 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG11 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG12 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG13 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG21 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG22 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG23 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG11 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG12 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG13 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG21 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG22 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG23 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG11 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG12 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG13 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG21 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG22 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG23 | 5        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG11 | 9        | 0.3           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG12 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG13 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG21 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG22 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG23 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG11 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG12 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG13 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG21 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG22 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG23 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG11 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG12 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG13 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG21 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG22 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG23 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG11 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG12 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG13 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG21 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG22 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG23 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG11 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG12 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG13 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG21 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG22 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG23 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG11 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG12 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG13 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG21 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG22 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG23 | 9        | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG11 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG12 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG13 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG21 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG22 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG23 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG11 | 11       | 0.3           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG12 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG13 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG21 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG22 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG23 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG11 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG12 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG13 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG21 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG22 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG23 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG11 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG12 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG13 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG21 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG22 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG23 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG11 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG12 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG13 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG21 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG22 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG23 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG11 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG12 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG13 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG21 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG22 | 11       | 0.3           |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG23 | 11       | 0.3           |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 12       | 0.3           |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 12       | 0.3           |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 12       | 0.3           |
| (1,876) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HD21 | 12       | 0.29          |
| (1,876) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HD21 | 12       | 0.29          |
| (1,876) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HD21 | 12       | 0.29          |
| (1,876) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HD21 | 12       | 0.29          |
| (1,876) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HD21 | 12       | 0.29          |
| (1,876) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HD21 | 12       | 0.29          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 16       | 0.29          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 16       | 0.29          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 16       | 0.29          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 16       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 16       | 0.29          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 16       | 0.29          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 16       | 0.29          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 16       | 0.29          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 16       | 0.29          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 19       | 0.29          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 19       | 0.29          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 19       | 0.29          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE21 | 15       | 0.28          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE22 | 15       | 0.28          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE21 | 15       | 0.28          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE22 | 15       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 17       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 17       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 17       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 17       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 17       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 17       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 17       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 17       | 0.28          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 17       | 0.28          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 11       | 0.28          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 11       | 0.28          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 11       | 0.28          |
| (1,449)  | 1:10:A:LEU:H    | 1:10:A:LEU:HD21 | 17       | 0.28          |
| (1,449)  | 1:10:A:LEU:H    | 1:10:A:LEU:HD22 | 17       | 0.28          |
| (1,449)  | 1:10:A:LEU:H    | 1:10:A:LEU:HD23 | 17       | 0.28          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 19       | 0.28          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 19       | 0.28          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 19       | 0.28          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE21 | 10       | 0.27          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE22 | 10       | 0.27          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE21 | 10       | 0.27          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE22 | 10       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 16       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,900)  | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 16       | 0.27          |
| (1,900)  | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 16       | 0.27          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 11       | 0.27          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 11       | 0.27          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 11       | 0.27          |
| (1,576)  | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 11       | 0.27          |
| (1,576)  | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 11       | 0.27          |
| (1,576)  | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 11       | 0.27          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE21 | 9        | 0.26          |
| (1,1069) | 1:67:A:LEU:HD11 | 1:71:A:GLN:HE22 | 9        | 0.26          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE21 | 9        | 0.26          |
| (1,1069) | 1:67:A:LEU:HD12 | 1:71:A:GLN:HE22 | 9        | 0.26          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE21 | 9        | 0.26          |
| (1,1069) | 1:67:A:LEU:HD13 | 1:71:A:GLN:HE22 | 9        | 0.26          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 4        | 0.26          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 4        | 0.26          |
| (1,681)  | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 4        | 0.26          |
| (1,426)  | 1:10:A:LEU:H    | 1:11:A:LYS:H    | 19       | 0.26          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 7        | 0.26          |
| (1,876)  | 1:17:A:VAL:HG11 | 1:57:A:ASN:HD21 | 8        | 0.25          |
| (1,876)  | 1:17:A:VAL:HG12 | 1:57:A:ASN:HD21 | 8        | 0.25          |
| (1,876)  | 1:17:A:VAL:HG13 | 1:57:A:ASN:HD21 | 8        | 0.25          |
| (1,876)  | 1:17:A:VAL:HG21 | 1:57:A:ASN:HD21 | 8        | 0.25          |
| (1,876)  | 1:17:A:VAL:HG22 | 1:57:A:ASN:HD21 | 8        | 0.25          |
| (1,876)  | 1:17:A:VAL:HG23 | 1:57:A:ASN:HD21 | 8        | 0.25          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 15       | 0.25          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 15       | 0.25          |
| (1,803)  | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 15       | 0.25          |
| (1,714)  | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 17       | 0.25          |
| (1,714)  | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 17       | 0.25          |
| (1,714)  | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 17       | 0.25          |
| (1,714)  | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 17       | 0.25          |
| (1,714)  | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 17       | 0.25          |
| (1,714)  | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 17       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,714)  | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 17       | 0.25          |
| (1,714)  | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 17       | 0.25          |
| (1,714)  | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 17       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 5        | 0.25          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 11       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 11       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 11       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 11       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 11       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 11       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 11       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 11       | 0.25          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 11       | 0.25          |
| (1,607)  | 1:42:A:THR:HB   | 1:58:A:PRO:HB3  | 16       | 0.25          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 17       | 0.25          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 17       | 0.25          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 17       | 0.25          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 6        | 0.25          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 6        | 0.25          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 6        | 0.25          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 7        | 0.25          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 7        | 0.25          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 7        | 0.25          |
| (1,67)   | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 18       | 0.25          |
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 18       | 0.25          |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 18       | 0.25          |
| (1,1075) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD2  | 2        | 0.24          |
| (1,1075) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD3  | 2        | 0.24          |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG2  | 2        | 0.24          |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 2        | 0.24          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG11 | 19       | 0.24          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG12 | 19       | 0.24          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG13 | 19       | 0.24          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 19       | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,992) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 19       | 0.24          |
| (1,992) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 19       | 0.24          |
| (1,876) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HD21 | 7        | 0.24          |
| (1,876) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HD21 | 7        | 0.24          |
| (1,876) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HD21 | 7        | 0.24          |
| (1,876) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HD21 | 7        | 0.24          |
| (1,876) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HD21 | 7        | 0.24          |
| (1,876) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HD21 | 7        | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG11 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG12 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG13 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG21 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG22 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG23 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG11 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG12 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG13 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG21 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG22 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG23 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG11 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG12 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG13 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG21 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG22 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG23 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG11 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG12 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG13 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG21 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG22 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG23 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG11 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG12 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG13 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG21 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG22 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG23 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG11 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG12 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG13 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG21 | 1        | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG22 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG23 | 1        | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG11 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG12 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG13 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG21 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG22 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG23 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG11 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG12 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG13 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG21 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG22 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG23 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG11 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG12 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG13 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG21 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG22 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG23 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG11 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG12 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG13 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG21 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG22 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG23 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG11 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG12 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG13 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG21 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG22 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG23 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG11 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG12 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG13 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG21 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG22 | 12       | 0.24          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG23 | 12       | 0.24          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 4        | 0.24          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 4        | 0.24          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 4        | 0.24          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 4        | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 4        | 0.24          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 4        | 0.24          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 4        | 0.24          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 4        | 0.24          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 4        | 0.24          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 14       | 0.24          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 14       | 0.24          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 14       | 0.24          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 14       | 0.24          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 14       | 0.24          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 14       | 0.24          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 14       | 0.24          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 14       | 0.24          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 14       | 0.24          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 20       | 0.24          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 20       | 0.24          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 20       | 0.24          |
| (1,67)   | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 11       | 0.24          |
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 11       | 0.24          |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 11       | 0.24          |
| (1,67)   | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 20       | 0.24          |
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 20       | 0.24          |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 20       | 0.24          |
| (1,1082) | 1:70:A:VAL:HG11 | 1:71:A:GLN:H    | 10       | 0.23          |
| (1,1082) | 1:70:A:VAL:HG12 | 1:71:A:GLN:H    | 10       | 0.23          |
| (1,1082) | 1:70:A:VAL:HG13 | 1:71:A:GLN:H    | 10       | 0.23          |
| (1,1082) | 1:70:A:VAL:HG21 | 1:71:A:GLN:H    | 10       | 0.23          |
| (1,1082) | 1:70:A:VAL:HG22 | 1:71:A:GLN:H    | 10       | 0.23          |
| (1,1082) | 1:70:A:VAL:HG23 | 1:71:A:GLN:H    | 10       | 0.23          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 10       | 0.23          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 10       | 0.23          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 10       | 0.23          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 10       | 0.23          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 10       | 0.23          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 10       | 0.23          |
| (1,1075) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD2  | 11       | 0.23          |
| (1,1075) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD3  | 11       | 0.23          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE2  | 17       | 0.23          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE3  | 17       | 0.23          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE2  | 17       | 0.23          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE3  | 17       | 0.23          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 20       | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 20       | 0.23          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 20       | 0.23          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 20       | 0.23          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 20       | 0.23          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 20       | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 1        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 4        | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 4        | 0.23          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 4        | 0.23          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 15       | 0.23          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 15       | 0.23          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 15       | 0.23          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 15       | 0.23          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 15       | 0.23          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 15       | 0.23          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG11 | 17       | 0.23          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG12 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG13 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG21 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG22 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD11 | 1:70:A:VAL:HG23 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG11 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG12 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG13 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG21 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG22 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG23 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG11 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG12 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG13 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG21 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG22 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG23 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG11 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG12 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG13 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG21 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG22 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG23 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG11 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG12 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG13 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG21 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG22 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG23 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG11 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG12 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG13 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG21 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG22 | 17       | 0.23          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG23 | 17       | 0.23          |
| (1,814) | 1:2:A:ILE:HG21 | 1:4:A:GLU:HG2   | 8        | 0.23          |
| (1,814) | 1:2:A:ILE:HG21 | 1:4:A:GLU:HG3   | 8        | 0.23          |
| (1,814) | 1:2:A:ILE:HG22 | 1:4:A:GLU:HG2   | 8        | 0.23          |
| (1,814) | 1:2:A:ILE:HG22 | 1:4:A:GLU:HG3   | 8        | 0.23          |
| (1,814) | 1:2:A:ILE:HG23 | 1:4:A:GLU:HG2   | 8        | 0.23          |
| (1,814) | 1:2:A:ILE:HG23 | 1:4:A:GLU:HG3   | 8        | 0.23          |
| (1,726) | 1:22:A:VAL:CG1 | 1:46:A:ILE:HD11 | 11       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD12 | 11       | 0.23          |
| (1,726)  | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD13 | 11       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 2        | 0.23          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 12       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 12       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 12       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 12       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 12       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 12       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 12       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 12       | 0.23          |
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 12       | 0.23          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 9        | 0.23          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 9        | 0.23          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 9        | 0.23          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 11       | 0.23          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 11       | 0.23          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 11       | 0.23          |
| (1,329)  | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 6        | 0.23          |
| (1,67)   | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 19       | 0.23          |
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 19       | 0.23          |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 19       | 0.23          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE21 | 13       | 0.22          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE22 | 13       | 0.22          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE21 | 13       | 0.22          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE22 | 13       | 0.22          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE21 | 16       | 0.22          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE22 | 16       | 0.22          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE21 | 16       | 0.22          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE22 | 16       | 0.22          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE2  | 18       | 0.22          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE3  | 18       | 0.22          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE2  | 18       | 0.22          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE3  | 18       | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 8        | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 8        | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 8        | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 8        | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 8        | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 8        | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 11       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 11       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 11       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 11       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 11       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 11       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 15       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 15       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 15       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 15       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 15       | 0.22          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 15       | 0.22          |
| (1,932) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 20       | 0.22          |
| (1,932) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 20       | 0.22          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 20       | 0.22          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 20       | 0.22          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 20       | 0.22          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 20       | 0.22          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 20       | 0.22          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 20       | 0.22          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 20       | 0.22          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 20       | 0.22          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 12       | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 12       | 0.22          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 12       | 0.22          |
| (1,876) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HD21 | 9        | 0.22          |
| (1,876) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HD21 | 9        | 0.22          |
| (1,876) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HD21 | 9        | 0.22          |
| (1,876) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HD21 | 9        | 0.22          |
| (1,876) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HD21 | 9        | 0.22          |
| (1,876) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HD21 | 9        | 0.22          |
| (1,814) | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG2   | 13       | 0.22          |
| (1,814) | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG3   | 13       | 0.22          |
| (1,814) | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG2   | 13       | 0.22          |
| (1,814) | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG3   | 13       | 0.22          |
| (1,814) | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG2   | 13       | 0.22          |
| (1,814) | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG3   | 13       | 0.22          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 19       | 0.22          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 20       | 0.22          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 20       | 0.22          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 20       | 0.22          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 20       | 0.22          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 20       | 0.22          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 20       | 0.22          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 20       | 0.22          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 20       | 0.22          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 20       | 0.22          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 18       | 0.22          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 18       | 0.22          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 18       | 0.22          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 18       | 0.22          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 18       | 0.22          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 18       | 0.22          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 18       | 0.22          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 18       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,707)  | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 18       | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 5        | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 5        | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 5        | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 6        | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 6        | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 6        | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 16       | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 16       | 0.22          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 16       | 0.22          |
| (1,586)  | 1:27:A:ILE:HD11 | 1:62:A:TRP:HZ3  | 10       | 0.22          |
| (1,586)  | 1:27:A:ILE:HD12 | 1:62:A:TRP:HZ3  | 10       | 0.22          |
| (1,586)  | 1:27:A:ILE:HD13 | 1:62:A:TRP:HZ3  | 10       | 0.22          |
| (1,329)  | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 11       | 0.22          |
| (1,329)  | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 15       | 0.22          |
| (1,329)  | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 18       | 0.22          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 6        | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 6        | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 6        | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 6        | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 6        | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 6        | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 16       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 16       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 16       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 16       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 16       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 16       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 20       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 20       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 20       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 20       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 20       | 0.21          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 20       | 0.21          |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG2  | 15       | 0.21          |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 15       | 0.21          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 2        | 0.21          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 2        | 0.21          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 2        | 0.21          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 2        | 0.21          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 2        | 0.21          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 2        | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 3        | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 3        | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 3        | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 3        | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 3        | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 3        | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 17       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 17       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 17       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 17       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 17       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 17       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 18       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 18       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 18       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 18       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 18       | 0.21          |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 18       | 0.21          |
| (1,948) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HB2  | 8        | 0.21          |
| (1,948) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HB3  | 8        | 0.21          |
| (1,948) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HB2  | 8        | 0.21          |
| (1,948) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HB3  | 8        | 0.21          |
| (1,948) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HB2  | 8        | 0.21          |
| (1,948) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HB3  | 8        | 0.21          |
| (1,884) | 1:21:A:VAL:HG11 | 1:62:A:TRP:HB2  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG11 | 1:62:A:TRP:HB3  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG12 | 1:62:A:TRP:HB2  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG12 | 1:62:A:TRP:HB3  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG13 | 1:62:A:TRP:HB2  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG13 | 1:62:A:TRP:HB3  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG21 | 1:62:A:TRP:HB2  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG21 | 1:62:A:TRP:HB3  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG22 | 1:62:A:TRP:HB2  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG22 | 1:62:A:TRP:HB3  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG23 | 1:62:A:TRP:HB2  | 3        | 0.21          |
| (1,884) | 1:21:A:VAL:HG23 | 1:62:A:TRP:HB3  | 3        | 0.21          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG11 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG12 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG13 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG21 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG22 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG23 | 16       | 0.21          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG11 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG12 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG13 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG21 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG22 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD12 | 1:70:A:VAL:HG23 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG11 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG12 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG13 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG21 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG22 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD13 | 1:70:A:VAL:HG23 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG11 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG12 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG13 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG21 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG22 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD21 | 1:70:A:VAL:HG23 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG11 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG12 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG13 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG21 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG22 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD22 | 1:70:A:VAL:HG23 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG11 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG12 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG13 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG21 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG22 | 16       | 0.21          |
| (1,825) | 1:3:A:LEU:HD23 | 1:70:A:VAL:HG23 | 16       | 0.21          |
| (1,814) | 1:2:A:ILE:HG21 | 1:4:A:GLU:HG2   | 20       | 0.21          |
| (1,814) | 1:2:A:ILE:HG21 | 1:4:A:GLU:HG3   | 20       | 0.21          |
| (1,814) | 1:2:A:ILE:HG22 | 1:4:A:GLU:HG2   | 20       | 0.21          |
| (1,814) | 1:2:A:ILE:HG22 | 1:4:A:GLU:HG3   | 20       | 0.21          |
| (1,814) | 1:2:A:ILE:HG23 | 1:4:A:GLU:HG2   | 20       | 0.21          |
| (1,814) | 1:2:A:ILE:HG23 | 1:4:A:GLU:HG3   | 20       | 0.21          |
| (1,717) | 1:4:A:GLU:HB3  | 1:31:A:GLN:HA   | 17       | 0.21          |
| (1,631) | 1:10:A:LEU:HA  | 1:10:A:LEU:HD21 | 19       | 0.21          |
| (1,631) | 1:10:A:LEU:HA  | 1:10:A:LEU:HD22 | 19       | 0.21          |
| (1,631) | 1:10:A:LEU:HA  | 1:10:A:LEU:HD23 | 19       | 0.21          |
| (1,620) | 1:66:A:LEU:HA  | 1:66:A:LEU:HD21 | 7        | 0.21          |
| (1,620) | 1:66:A:LEU:HA  | 1:66:A:LEU:HD22 | 7        | 0.21          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,620)  | 1:66:A:LEU:HA  | 1:66:A:LEU:HD23 | 7        | 0.21          |
| (1,449)  | 1:10:A:LEU:H   | 1:10:A:LEU:HD21 | 1        | 0.21          |
| (1,449)  | 1:10:A:LEU:H   | 1:10:A:LEU:HD22 | 1        | 0.21          |
| (1,449)  | 1:10:A:LEU:H   | 1:10:A:LEU:HD23 | 1        | 0.21          |
| (1,329)  | 1:4:A:GLU:HB2  | 1:31:A:GLN:HA   | 3        | 0.21          |
| (1,329)  | 1:4:A:GLU:HB2  | 1:31:A:GLN:HA   | 12       | 0.21          |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG11 | 13       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG12 | 13       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG13 | 13       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG21 | 13       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG22 | 13       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG23 | 13       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG11 | 15       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG12 | 15       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG13 | 15       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG21 | 15       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG22 | 15       | 0.2           |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG23 | 15       | 0.2           |
| (1,974)  | 1:41:A:LYS:HB2 | 1:41:A:LYS:HE2  | 12       | 0.2           |
| (1,974)  | 1:41:A:LYS:HB2 | 1:41:A:LYS:HE3  | 12       | 0.2           |
| (1,974)  | 1:41:A:LYS:HB3 | 1:41:A:LYS:HE2  | 12       | 0.2           |
| (1,974)  | 1:41:A:LYS:HB3 | 1:41:A:LYS:HE3  | 12       | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG11 | 6        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG12 | 6        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG13 | 6        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG21 | 6        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG22 | 6        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG23 | 6        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG11 | 9        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG12 | 9        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG13 | 9        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG21 | 9        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG22 | 9        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG23 | 9        | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG11 | 12       | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG12 | 12       | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG13 | 12       | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG21 | 12       | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG22 | 12       | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG23 | 12       | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG11 | 13       | 0.2           |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG12 | 13       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 13       | 0.2           |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 13       | 0.2           |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 13       | 0.2           |
| (1,955) | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 10       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 13       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 13       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 20       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 20       | 0.2           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 20       | 0.2           |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 5        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 5        | 0.2           |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 5        | 0.2           |
| (1,841) | 1:9:A:ASN:HB2   | 1:10:A:LEU:H    | 3        | 0.2           |
| (1,841) | 1:9:A:ASN:HB3   | 1:10:A:LEU:H    | 3        | 0.2           |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 10       | 0.2           |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 10       | 0.2           |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 10       | 0.2           |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 13       | 0.2           |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 20       | 0.2           |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 20       | 0.2           |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 20       | 0.2           |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 20       | 0.2           |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 20       | 0.2           |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 20       | 0.2           |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 20       | 0.2           |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 20       | 0.2           |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 20       | 0.2           |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 3        | 0.2           |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 3        | 0.2           |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 3        | 0.2           |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD21 | 16       | 0.2           |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD22 | 16       | 0.2           |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD23 | 16       | 0.2           |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 2        | 0.2           |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 2        | 0.2           |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 2        | 0.2           |
| (1,449) | 1:10:A:LEU:H    | 1:10:A:LEU:HD21 | 6        | 0.2           |
| (1,449) | 1:10:A:LEU:H    | 1:10:A:LEU:HD22 | 6        | 0.2           |
| (1,449) | 1:10:A:LEU:H    | 1:10:A:LEU:HD23 | 6        | 0.2           |
| (1,445) | 1:4:A:GLU:H     | 1:4:A:GLU:HG2   | 18       | 0.2           |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 13       | 0.2           |
| (1,263) | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 13       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 13       | 0.2           |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 12       | 0.2           |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 12       | 0.2           |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 12       | 0.2           |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 4        | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 4        | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 4        | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 4        | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 4        | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 4        | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 11       | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 11       | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 11       | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 11       | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 11       | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 11       | 0.19          |
| (1,1075) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD2  | 18       | 0.19          |
| (1,1075) | 1:68:A:ARG:HA   | 1:68:A:ARG:HD3  | 18       | 0.19          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE2  | 8        | 0.19          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE3  | 8        | 0.19          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE2  | 8        | 0.19          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE3  | 8        | 0.19          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE2  | 15       | 0.19          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE3  | 15       | 0.19          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE2  | 15       | 0.19          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE3  | 15       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD11 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD12 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD13 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD21 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD22 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD23 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD11 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD12 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD13 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD21 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD22 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD23 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD11 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD12 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD13 | 16       | 0.19          |
| (1,925)  | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD21 | 16       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD22 | 16       | 0.19          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD23 | 16       | 0.19          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 8        | 0.19          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG11 | 1:62:A:TRP:HB2  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG11 | 1:62:A:TRP:HB3  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG12 | 1:62:A:TRP:HB2  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG12 | 1:62:A:TRP:HB3  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG13 | 1:62:A:TRP:HB2  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG13 | 1:62:A:TRP:HB3  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG21 | 1:62:A:TRP:HB2  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG21 | 1:62:A:TRP:HB3  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG22 | 1:62:A:TRP:HB2  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG22 | 1:62:A:TRP:HB3  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG23 | 1:62:A:TRP:HB2  | 8        | 0.19          |
| (1,884) | 1:21:A:VAL:HG23 | 1:62:A:TRP:HB3  | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 8        | 0.19          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 11       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 11       | 0.19          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 11       | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 11       | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 11       | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 11       | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 11       | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 11       | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 11       | 0.19          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 15       | 0.19          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 15       | 0.19          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 15       | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 15       | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 15       | 0.19          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 15       | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 15       | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 15       | 0.19          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 15       | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 1        | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 7        | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 19       | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 19       | 0.19          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 19       | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 19       | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 19       | 0.19          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 19       | 0.19          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 19       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 19       | 0.19          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 19       | 0.19          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 13       | 0.19          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 13       | 0.19          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 13       | 0.19          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 19       | 0.19          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 19       | 0.19          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 19       | 0.19          |
| (1,673) | 1:42:A:THR:HB   | 1:58:A:PRO:HG3  | 12       | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD21 | 5        | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD22 | 5        | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD23 | 5        | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD21 | 8        | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD22 | 8        | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD23 | 8        | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD21 | 15       | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD22 | 15       | 0.19          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD23 | 15       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 13       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 13       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 13       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 15       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 15       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 15       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 16       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 16       | 0.19          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 16       | 0.19          |
| (1,586) | 1:27:A:ILE:HD11 | 1:62:A:TRP:HZ3  | 16       | 0.19          |
| (1,586) | 1:27:A:ILE:HD12 | 1:62:A:TRP:HZ3  | 16       | 0.19          |
| (1,586) | 1:27:A:ILE:HD13 | 1:62:A:TRP:HZ3  | 16       | 0.19          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 12       | 0.19          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 12       | 0.19          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 12       | 0.19          |
| (1,445) | 1:4:A:GLU:H     | 1:4:A:GLU:HG2   | 11       | 0.19          |
| (1,239) | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 15       | 0.19          |
| (1,239) | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 15       | 0.19          |
| (1,239) | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 15       | 0.19          |
| (1,239) | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 16       | 0.19          |
| (1,239) | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 16       | 0.19          |
| (1,239) | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 16       | 0.19          |
| (1,118) | 1:35:A:PRO:HB2  | 1:36:A:GLY:H    | 11       | 0.19          |
| (1,67)  | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 9        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 9        | 0.19          |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 9        | 0.19          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 1        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 1        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 1        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 1        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 1        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 1        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 2        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 2        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 2        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 2        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 2        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 2        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 3        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 3        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 3        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 3        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 3        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 3        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 5        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 5        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 5        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 5        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 5        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 5        | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 12       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 12       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 12       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 12       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 12       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 12       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 18       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 18       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 18       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 18       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 18       | 0.18          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 18       | 0.18          |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG2  | 17       | 0.18          |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 17       | 0.18          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD11 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD12 | 4        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD13 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD21 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD22 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD23 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD11 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD12 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD13 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD21 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD22 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD23 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD11 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD12 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD13 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD21 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD22 | 4        | 0.18          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD23 | 4        | 0.18          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG11 | 17       | 0.18          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG12 | 17       | 0.18          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG13 | 17       | 0.18          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 17       | 0.18          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 17       | 0.18          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 17       | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 7        | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 7        | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 7        | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 7        | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 7        | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 7        | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 16       | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 16       | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 16       | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG21 | 16       | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG22 | 16       | 0.18          |
| (1,955)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG23 | 16       | 0.18          |
| (1,948)  | 1:30:A:ILE:HD11 | 1:66:A:LEU:HB2  | 10       | 0.18          |
| (1,948)  | 1:30:A:ILE:HD11 | 1:66:A:LEU:HB3  | 10       | 0.18          |
| (1,948)  | 1:30:A:ILE:HD12 | 1:66:A:LEU:HB2  | 10       | 0.18          |
| (1,948)  | 1:30:A:ILE:HD12 | 1:66:A:LEU:HB3  | 10       | 0.18          |
| (1,948)  | 1:30:A:ILE:HD13 | 1:66:A:LEU:HB2  | 10       | 0.18          |
| (1,948)  | 1:30:A:ILE:HD13 | 1:66:A:LEU:HB3  | 10       | 0.18          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 6        | 0.18          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 6        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 6        | 0.18          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 6        | 0.18          |
| (1,932) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 11       | 0.18          |
| (1,932) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 11       | 0.18          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 11       | 0.18          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 11       | 0.18          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 6        | 0.18          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 6        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,867) | 1:17:A:VAL:HG11 | 1:55:A:CYS:CB   | 15       | 0.18          |
| (1,867) | 1:17:A:VAL:HG12 | 1:55:A:CYS:CB   | 15       | 0.18          |
| (1,867) | 1:17:A:VAL:HG13 | 1:55:A:CYS:CB   | 15       | 0.18          |
| (1,867) | 1:17:A:VAL:HG21 | 1:55:A:CYS:CB   | 15       | 0.18          |
| (1,867) | 1:17:A:VAL:HG22 | 1:55:A:CYS:CB   | 15       | 0.18          |
| (1,867) | 1:17:A:VAL:HG23 | 1:55:A:CYS:CB   | 15       | 0.18          |
| (1,814) | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG2   | 10       | 0.18          |
| (1,814) | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG3   | 10       | 0.18          |
| (1,814) | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG2   | 10       | 0.18          |
| (1,814) | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG3   | 10       | 0.18          |
| (1,814) | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG2   | 10       | 0.18          |
| (1,814) | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG3   | 10       | 0.18          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG21 | 7        | 0.18          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG22 | 7        | 0.18          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG23 | 7        | 0.18          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 1        | 0.18          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 1        | 0.18          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 1        | 0.18          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 1        | 0.18          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 1        | 0.18          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 1        | 0.18          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 1        | 0.18          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 1        | 0.18          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 1        | 0.18          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 6        | 0.18          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 10       | 0.18          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 10       | 0.18          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 10       | 0.18          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 10       | 0.18          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 10       | 0.18          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 10       | 0.18          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 10       | 0.18          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 10       | 0.18          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 10       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG11 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG12 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG13 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG11 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG12 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG13 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG11 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG12 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG13 | 8        | 0.18          |
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG11 | 20       | 0.18          |
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG12 | 20       | 0.18          |
| (1,704)  | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG13 | 20       | 0.18          |
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG11 | 20       | 0.18          |
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG12 | 20       | 0.18          |
| (1,704)  | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG13 | 20       | 0.18          |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG11 | 20       | 0.18          |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG12 | 20       | 0.18          |
| (1,704)  | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG13 | 20       | 0.18          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 14       | 0.18          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 14       | 0.18          |
| (1,676)  | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 14       | 0.18          |
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 4        | 0.18          |
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 4        | 0.18          |
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 4        | 0.18          |
| (1,604)  | 1:22:A:VAL:HB   | 1:62:A:TRP:HH2  | 10       | 0.18          |
| (1,494)  | 1:46:A:ILE:H    | 1:55:A:CYS:HA   | 3        | 0.18          |
| (1,484)  | 1:37:A:ASN:HB3  | 1:38:A:GLY:H    | 5        | 0.18          |
| (1,459)  | 1:13:A:ARG:H    | 1:13:A:ARG:HG2  | 17       | 0.18          |
| (1,263)  | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 7        | 0.18          |
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 7        | 0.18          |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 7        | 0.18          |
| (1,255)  | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 6        | 0.18          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 10       | 0.18          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 10       | 0.18          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 10       | 0.18          |
| (1,11)   | 1:36:A:GLY:H    | 1:39:A:CYS:H    | 12       | 0.18          |
| (3,19)   | 1:33:A:THR:O    | 1:43:A:GLU:H    | 9        | 0.17          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE21 | 17       | 0.17          |
| (1,1084) | 1:71:A:GLN:HB2  | 1:71:A:GLN:HE22 | 17       | 0.17          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE21 | 17       | 0.17          |
| (1,1084) | 1:71:A:GLN:HB3  | 1:71:A:GLN:HE22 | 17       | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 8        | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 8        | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 8        | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 8        | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 8        | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 14       | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 14       | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 14       | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 14       | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 14       | 0.17          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 14       | 0.17          |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG2  | 12       | 0.17          |
| (1,1042) | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 12       | 0.17          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE2  | 11       | 0.17          |
| (1,974)  | 1:41:A:LYS:HB2  | 1:41:A:LYS:HE3  | 11       | 0.17          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE2  | 11       | 0.17          |
| (1,974)  | 1:41:A:LYS:HB3  | 1:41:A:LYS:HE3  | 11       | 0.17          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 19       | 0.17          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 19       | 0.17          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 19       | 0.17          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 19       | 0.17          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 19       | 0.17          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 19       | 0.17          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 19       | 0.17          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 19       | 0.17          |
| (1,876)  | 1:17:A:VAL:HG11 | 1:57:A:ASN:HD21 | 13       | 0.17          |
| (1,876)  | 1:17:A:VAL:HG12 | 1:57:A:ASN:HD21 | 13       | 0.17          |
| (1,876)  | 1:17:A:VAL:HG13 | 1:57:A:ASN:HD21 | 13       | 0.17          |
| (1,876)  | 1:17:A:VAL:HG21 | 1:57:A:ASN:HD21 | 13       | 0.17          |
| (1,876)  | 1:17:A:VAL:HG22 | 1:57:A:ASN:HD21 | 13       | 0.17          |
| (1,876)  | 1:17:A:VAL:HG23 | 1:57:A:ASN:HD21 | 13       | 0.17          |
| (1,814)  | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG2   | 19       | 0.17          |
| (1,814)  | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG3   | 19       | 0.17          |
| (1,814)  | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG2   | 19       | 0.17          |
| (1,814)  | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG3   | 19       | 0.17          |
| (1,814)  | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG2   | 19       | 0.17          |
| (1,814)  | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG3   | 19       | 0.17          |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD11 | 3        | 0.17          |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD12 | 3        | 0.17          |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD13 | 3        | 0.17          |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD21 | 3        | 0.17          |
| (1,812)  | 1:1:A:MET:HE1   | 1:66:A:LEU:HD22 | 3        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD23 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD11 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD12 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD13 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD21 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD22 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD23 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD11 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD12 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD13 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD21 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD22 | 3        | 0.17          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD23 | 3        | 0.17          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 9        | 0.17          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 9        | 0.17          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 9        | 0.17          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 9        | 0.17          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 9        | 0.17          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 9        | 0.17          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 9        | 0.17          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 9        | 0.17          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 9        | 0.17          |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD21 | 19       | 0.17          |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD22 | 19       | 0.17          |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD23 | 19       | 0.17          |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD21 | 19       | 0.17          |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD22 | 19       | 0.17          |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD23 | 19       | 0.17          |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD21 | 19       | 0.17          |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD22 | 19       | 0.17          |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD23 | 19       | 0.17          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 10       | 0.17          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 10       | 0.17          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 10       | 0.17          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 12       | 0.17          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 12       | 0.17          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 12       | 0.17          |
| (1,673) | 1:42:A:THR:HB   | 1:58:A:PRO:HG3  | 18       | 0.17          |
| (1,645) | 1:61:A:LYS:HA   | 1:61:A:LYS:HD2  | 17       | 0.17          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD21 | 18       | 0.17          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD22 | 18       | 0.17          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD23 | 18       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 18       | 0.17          |
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 18       | 0.17          |
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 18       | 0.17          |
| (1,619)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD21 | 9        | 0.17          |
| (1,619)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD22 | 9        | 0.17          |
| (1,619)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD23 | 9        | 0.17          |
| (1,453)  | 1:11:A:LYS:H    | 1:11:A:LYS:HG2  | 15       | 0.17          |
| (1,452)  | 1:8:A:THR:HG21  | 1:9:A:ASN:H     | 6        | 0.17          |
| (1,452)  | 1:8:A:THR:HG22  | 1:9:A:ASN:H     | 6        | 0.17          |
| (1,452)  | 1:8:A:THR:HG23  | 1:9:A:ASN:H     | 6        | 0.17          |
| (1,329)  | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 9        | 0.17          |
| (1,263)  | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 5        | 0.17          |
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 5        | 0.17          |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 5        | 0.17          |
| (1,255)  | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 10       | 0.17          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 4        | 0.17          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 4        | 0.17          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 4        | 0.17          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 18       | 0.17          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 18       | 0.17          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 18       | 0.17          |
| (1,223)  | 1:67:A:LEU:HA   | 1:71:A:GLN:H    | 15       | 0.17          |
| (1,67)   | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 16       | 0.17          |
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 16       | 0.17          |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 16       | 0.17          |
| (1,1083) | 1:71:A:GLN:H    | 1:71:A:GLN:HG2  | 1        | 0.16          |
| (1,1083) | 1:71:A:GLN:H    | 1:71:A:GLN:HG3  | 1        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 7        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 7        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 7        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 7        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 7        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 7        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 9        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 9        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 9        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 9        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG22 | 9        | 0.16          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG23 | 9        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD11 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD12 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD13 | 7        | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD21 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD22 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HD23 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD11 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD12 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD13 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD21 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD22 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HD23 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD11 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD12 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD13 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD21 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD22 | 7        | 0.16          |
| (1,1040) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HD23 | 7        | 0.16          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 3        | 0.16          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 3        | 0.16          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 9        | 0.16          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 9        | 0.16          |
| (1,950)  | 1:30:A:ILE:HD11 | 1:70:A:VAL:HG11 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD11 | 1:70:A:VAL:HG12 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD11 | 1:70:A:VAL:HG13 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD11 | 1:70:A:VAL:HG21 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD11 | 1:70:A:VAL:HG22 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD11 | 1:70:A:VAL:HG23 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD12 | 1:70:A:VAL:HG11 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD12 | 1:70:A:VAL:HG12 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD12 | 1:70:A:VAL:HG13 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD12 | 1:70:A:VAL:HG21 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD12 | 1:70:A:VAL:HG22 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD12 | 1:70:A:VAL:HG23 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD13 | 1:70:A:VAL:HG11 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD13 | 1:70:A:VAL:HG12 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD13 | 1:70:A:VAL:HG13 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD13 | 1:70:A:VAL:HG21 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD13 | 1:70:A:VAL:HG22 | 12       | 0.16          |
| (1,950)  | 1:30:A:ILE:HD13 | 1:70:A:VAL:HG23 | 12       | 0.16          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 8        | 0.16          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 8        | 0.16          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 8        | 0.16          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 8        | 0.16          |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 8        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 8        | 0.16          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 8        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 4        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 4        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 4        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 4        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 4        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 4        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 6        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 6        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 6        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 6        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 6        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 6        | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 16       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 16       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 16       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 16       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 16       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 16       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 18       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 18       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 18       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 18       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 18       | 0.16          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 18       | 0.16          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 1        | 0.16          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 1        | 0.16          |
| (1,875) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HB3  | 16       | 0.16          |
| (1,875) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HB3  | 16       | 0.16          |
| (1,875) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HB3  | 16       | 0.16          |
| (1,875) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HB3  | 16       | 0.16          |
| (1,875) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HB3  | 16       | 0.16          |
| (1,875) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HB3  | 16       | 0.16          |
| (1,835) | 1:4:A:GLU:HB2   | 1:31:A:GLN:HG3  | 1        | 0.16          |
| (1,835) | 1:4:A:GLU:HB3   | 1:31:A:GLN:HG3  | 1        | 0.16          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG11 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG12 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG13 | 18       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG21 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG22 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD11  | 1:70:A:VAL:HG23 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG11 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG12 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG13 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG21 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG22 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD12  | 1:70:A:VAL:HG23 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG11 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG12 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG13 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG21 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG22 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD13  | 1:70:A:VAL:HG23 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG11 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG12 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG13 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG21 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG22 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD21  | 1:70:A:VAL:HG23 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG11 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG12 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG13 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG21 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG22 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD22  | 1:70:A:VAL:HG23 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG11 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG12 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG13 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG21 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG22 | 18       | 0.16          |
| (1,825) | 1:3:A:LEU:HD23  | 1:70:A:VAL:HG23 | 18       | 0.16          |
| (1,814) | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG2   | 16       | 0.16          |
| (1,814) | 1:2:A:ILE:HG21  | 1:4:A:GLU:HG3   | 16       | 0.16          |
| (1,814) | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG2   | 16       | 0.16          |
| (1,814) | 1:2:A:ILE:HG22  | 1:4:A:GLU:HG3   | 16       | 0.16          |
| (1,814) | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG2   | 16       | 0.16          |
| (1,814) | 1:2:A:ILE:HG23  | 1:4:A:GLU:HG3   | 16       | 0.16          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 4        | 0.16          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 4        | 0.16          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 4        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 4        | 0.16          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 4        | 0.16          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 4        | 0.16          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 4        | 0.16          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 4        | 0.16          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 4        | 0.16          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 6        | 0.16          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 6        | 0.16          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 6        | 0.16          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 6        | 0.16          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 6        | 0.16          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 6        | 0.16          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 6        | 0.16          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 6        | 0.16          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 6        | 0.16          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 3        | 0.16          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 9        | 0.16          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 9        | 0.16          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 9        | 0.16          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 9        | 0.16          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 9        | 0.16          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 9        | 0.16          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 9        | 0.16          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 9        | 0.16          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 9        | 0.16          |
| (1,644) | 1:26:A:ILE:HA   | 1:49:A:LYS:HB2  | 2        | 0.16          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 1        | 0.16          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 1        | 0.16          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 1        | 0.16          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 5        | 0.16          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 5        | 0.16          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 5        | 0.16          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD21 | 17       | 0.16          |
| (1,620) | 1:66:A:LEU:HA   | 1:66:A:LEU:HD22 | 17       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,620)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD23 | 17       | 0.16          |
| (1,604)  | 1:22:A:VAL:HB   | 1:62:A:TRP:HH2  | 3        | 0.16          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 6        | 0.16          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 6        | 0.16          |
| (1,497)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 6        | 0.16          |
| (1,453)  | 1:11:A:LYS:H    | 1:11:A:LYS:HG2  | 10       | 0.16          |
| (1,446)  | 1:4:A:GLU:H     | 1:4:A:GLU:HG3   | 13       | 0.16          |
| (1,426)  | 1:10:A:LEU:H    | 1:11:A:LYS:H    | 3        | 0.16          |
| (1,329)  | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 16       | 0.16          |
| (1,289)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD11 | 7        | 0.16          |
| (1,289)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD12 | 7        | 0.16          |
| (1,289)  | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD13 | 7        | 0.16          |
| (1,285)  | 1:44:A:VAL:HG21 | 1:58:A:PRO:HB3  | 1        | 0.16          |
| (1,285)  | 1:44:A:VAL:HG22 | 1:58:A:PRO:HB3  | 1        | 0.16          |
| (1,285)  | 1:44:A:VAL:HG23 | 1:58:A:PRO:HB3  | 1        | 0.16          |
| (1,263)  | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 18       | 0.16          |
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 18       | 0.16          |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 18       | 0.16          |
| (1,254)  | 1:57:A:ASN:HD22 | 1:60:A:ALA:HA   | 14       | 0.16          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 14       | 0.16          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 14       | 0.16          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 14       | 0.16          |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD21 | 8        | 0.16          |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD22 | 8        | 0.16          |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD23 | 8        | 0.16          |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD21 | 10       | 0.16          |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD22 | 10       | 0.16          |
| (1,216)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD23 | 10       | 0.16          |
| (1,67)   | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 8        | 0.16          |
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 8        | 0.16          |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 8        | 0.16          |
| (3,19)   | 1:33:A:THR:O    | 1:43:A:GLU:H    | 13       | 0.15          |
| (1,1082) | 1:70:A:VAL:HG11 | 1:71:A:GLN:H    | 20       | 0.15          |
| (1,1082) | 1:70:A:VAL:HG12 | 1:71:A:GLN:H    | 20       | 0.15          |
| (1,1082) | 1:70:A:VAL:HG13 | 1:71:A:GLN:H    | 20       | 0.15          |
| (1,1082) | 1:70:A:VAL:HG21 | 1:71:A:GLN:H    | 20       | 0.15          |
| (1,1082) | 1:70:A:VAL:HG22 | 1:71:A:GLN:H    | 20       | 0.15          |
| (1,1082) | 1:70:A:VAL:HG23 | 1:71:A:GLN:H    | 20       | 0.15          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG11 | 17       | 0.15          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG12 | 17       | 0.15          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG13 | 17       | 0.15          |
| (1,1081) | 1:70:A:VAL:H    | 1:70:A:VAL:HG21 | 17       | 0.15          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG22 | 17       | 0.15          |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG23 | 17       | 0.15          |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG11 | 19       | 0.15          |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG12 | 19       | 0.15          |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG13 | 19       | 0.15          |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG21 | 19       | 0.15          |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG22 | 19       | 0.15          |
| (1,1081) | 1:70:A:VAL:H   | 1:70:A:VAL:HG23 | 19       | 0.15          |
| (1,1077) | 1:68:A:ARG:HA  | 1:71:A:GLN:HE21 | 10       | 0.15          |
| (1,1077) | 1:68:A:ARG:HA  | 1:71:A:GLN:HE22 | 10       | 0.15          |
| (1,1038) | 1:63:A:LEU:HA  | 1:66:A:LEU:HD11 | 10       | 0.15          |
| (1,1038) | 1:63:A:LEU:HA  | 1:66:A:LEU:HD12 | 10       | 0.15          |
| (1,1038) | 1:63:A:LEU:HA  | 1:66:A:LEU:HD13 | 10       | 0.15          |
| (1,1038) | 1:63:A:LEU:HA  | 1:66:A:LEU:HD21 | 10       | 0.15          |
| (1,1038) | 1:63:A:LEU:HA  | 1:66:A:LEU:HD22 | 10       | 0.15          |
| (1,1038) | 1:63:A:LEU:HA  | 1:66:A:LEU:HD23 | 10       | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG11 | 7        | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG12 | 7        | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG13 | 7        | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG21 | 7        | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG22 | 7        | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG23 | 7        | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG11 | 20       | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG12 | 20       | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG13 | 20       | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG21 | 20       | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG22 | 20       | 0.15          |
| (1,991)  | 1:47:A:TRP:HD1 | 1:53:A:VAL:HG23 | 20       | 0.15          |
| (1,963)  | 1:33:A:THR:HA  | 1:34:A:PRO:HD2  | 12       | 0.15          |
| (1,963)  | 1:33:A:THR:HA  | 1:34:A:PRO:HD3  | 12       | 0.15          |
| (1,963)  | 1:33:A:THR:HA  | 1:34:A:PRO:HD2  | 14       | 0.15          |
| (1,963)  | 1:33:A:THR:HA  | 1:34:A:PRO:HD3  | 14       | 0.15          |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG11 | 4        | 0.15          |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG12 | 4        | 0.15          |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG13 | 4        | 0.15          |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG21 | 4        | 0.15          |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG22 | 4        | 0.15          |
| (1,955)  | 1:32:A:VAL:H   | 1:32:A:VAL:HG23 | 4        | 0.15          |
| (1,932)  | 1:28:A:ASP:HB2 | 1:49:A:LYS:HG2  | 7        | 0.15          |
| (1,932)  | 1:28:A:ASP:HB2 | 1:49:A:LYS:HG3  | 7        | 0.15          |
| (1,932)  | 1:28:A:ASP:HB3 | 1:49:A:LYS:HG2  | 7        | 0.15          |
| (1,932)  | 1:28:A:ASP:HB3 | 1:49:A:LYS:HG3  | 7        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD11 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD12 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD13 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD21 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD22 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD23 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD11 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD12 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD13 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD21 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD22 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD23 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD11 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD12 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD13 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD21 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD22 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD23 | 5        | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD11 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD12 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD13 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD21 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD22 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD23 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD11 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD12 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD13 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD21 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD22 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD23 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD11 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD12 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD13 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD21 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD22 | 11       | 0.15          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD23 | 11       | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 2        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 2        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 2        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 2        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 2        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 2        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 9        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 9        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 9        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 9        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 9        | 0.15          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 9        | 0.15          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 9        | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 4        | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 4        | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 4        | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 4        | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 4        | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 4        | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 14       | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 14       | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 14       | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 14       | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 14       | 0.15          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 14       | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD11 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD12 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD13 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD21 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD22 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD23 | 8        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD11 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD12 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD13 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD21 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD22 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD23 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD11 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD12 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD13 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD21 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD22 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD23 | 8        | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD11 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD12 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD13 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD21 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD22 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD23 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD11 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD12 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD13 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD21 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD22 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD23 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD11 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD12 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD13 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD21 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD22 | 17       | 0.15          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD23 | 17       | 0.15          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 2        | 0.15          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 18       | 0.15          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 18       | 0.15          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 18       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 18       | 0.15          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 18       | 0.15          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 18       | 0.15          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 18       | 0.15          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 18       | 0.15          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 18       | 0.15          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD21 | 8        | 0.15          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD22 | 8        | 0.15          |
| (1,707) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD23 | 8        | 0.15          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD21 | 8        | 0.15          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD22 | 8        | 0.15          |
| (1,707) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD23 | 8        | 0.15          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD21 | 8        | 0.15          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD22 | 8        | 0.15          |
| (1,707) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD23 | 8        | 0.15          |
| (1,704) | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG11 | 12       | 0.15          |
| (1,704) | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG12 | 12       | 0.15          |
| (1,704) | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG13 | 12       | 0.15          |
| (1,704) | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG11 | 12       | 0.15          |
| (1,704) | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG12 | 12       | 0.15          |
| (1,704) | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG13 | 12       | 0.15          |
| (1,704) | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG11 | 12       | 0.15          |
| (1,704) | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG12 | 12       | 0.15          |
| (1,704) | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG13 | 12       | 0.15          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 6        | 0.15          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 6        | 0.15          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 6        | 0.15          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG21 | 20       | 0.15          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG22 | 20       | 0.15          |
| (1,681) | 1:44:A:VAL:HB   | 1:56:A:VAL:HG23 | 20       | 0.15          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 2        | 0.15          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 2        | 0.15          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 2        | 0.15          |
| (1,645) | 1:61:A:LYS:HA   | 1:61:A:LYS:HD2  | 18       | 0.15          |
| (1,608) | 1:42:A:THR:HB   | 1:58:A:PRO:HB2  | 10       | 0.15          |
| (1,604) | 1:22:A:VAL:HB   | 1:62:A:TRP:HH2  | 9        | 0.15          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 13       | 0.15          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 13       | 0.15          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 13       | 0.15          |
| (1,453) | 1:11:A:LYS:H    | 1:11:A:LYS:HG2  | 13       | 0.15          |
| (1,350) | 1:18:A:ILE:HB   | 1:54:A:ILE:HG21 | 17       | 0.15          |
| (1,350) | 1:18:A:ILE:HB   | 1:54:A:ILE:HG22 | 17       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,350)  | 1:18:A:ILE:HB   | 1:54:A:ILE:HG23 | 17       | 0.15          |
| (1,343)  | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 18       | 0.15          |
| (1,343)  | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 18       | 0.15          |
| (1,343)  | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 18       | 0.15          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD11 | 8        | 0.15          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD12 | 8        | 0.15          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD13 | 8        | 0.15          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD11 | 20       | 0.15          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD12 | 20       | 0.15          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD13 | 20       | 0.15          |
| (1,255)  | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 9        | 0.15          |
| (1,255)  | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 11       | 0.15          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 1        | 0.15          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 1        | 0.15          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 1        | 0.15          |
| (1,67)   | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 17       | 0.15          |
| (1,67)   | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 17       | 0.15          |
| (1,67)   | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 17       | 0.15          |
| (1,2)    | 1:13:A:ARG:H    | 1:14:A:CYS:H    | 19       | 0.15          |
| (1,1082) | 1:70:A:VAL:HG11 | 1:71:A:GLN:H    | 16       | 0.14          |
| (1,1082) | 1:70:A:VAL:HG12 | 1:71:A:GLN:H    | 16       | 0.14          |
| (1,1082) | 1:70:A:VAL:HG13 | 1:71:A:GLN:H    | 16       | 0.14          |
| (1,1082) | 1:70:A:VAL:HG21 | 1:71:A:GLN:H    | 16       | 0.14          |
| (1,1082) | 1:70:A:VAL:HG22 | 1:71:A:GLN:H    | 16       | 0.14          |
| (1,1082) | 1:70:A:VAL:HG23 | 1:71:A:GLN:H    | 16       | 0.14          |
| (1,1077) | 1:68:A:ARG:HA   | 1:71:A:GLN:HE21 | 1        | 0.14          |
| (1,1077) | 1:68:A:ARG:HA   | 1:71:A:GLN:HE22 | 1        | 0.14          |
| (1,1052) | 1:65:A:ARG:H    | 1:65:A:ARG:HD2  | 5        | 0.14          |
| (1,1052) | 1:65:A:ARG:H    | 1:65:A:ARG:HD3  | 5        | 0.14          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 7        | 0.14          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 7        | 0.14          |
| (1,924)  | 1:27:A:ILE:HG21 | 1:30:A:ILE:HG12 | 17       | 0.14          |
| (1,924)  | 1:27:A:ILE:HG21 | 1:30:A:ILE:HG13 | 17       | 0.14          |
| (1,924)  | 1:27:A:ILE:HG22 | 1:30:A:ILE:HG12 | 17       | 0.14          |
| (1,924)  | 1:27:A:ILE:HG22 | 1:30:A:ILE:HG13 | 17       | 0.14          |
| (1,924)  | 1:27:A:ILE:HG23 | 1:30:A:ILE:HG12 | 17       | 0.14          |
| (1,924)  | 1:27:A:ILE:HG23 | 1:30:A:ILE:HG13 | 17       | 0.14          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 8        | 0.14          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 8        | 0.14          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 8        | 0.14          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 8        | 0.14          |
| (1,909)  | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 8        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 8        | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 11       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 11       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 11       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 11       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 11       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 11       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 12       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 12       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 12       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 12       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 12       | 0.14          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 12       | 0.14          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 2        | 0.14          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 20       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 20       | 0.14          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 20       | 0.14          |
| (1,875) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HB3  | 15       | 0.14          |
| (1,875) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HB3  | 15       | 0.14          |
| (1,875) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HB3  | 15       | 0.14          |
| (1,875) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HB3  | 15       | 0.14          |
| (1,875) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HB3  | 15       | 0.14          |
| (1,875) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HB3  | 15       | 0.14          |
| (1,875) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HB3  | 19       | 0.14          |
| (1,875) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HB3  | 19       | 0.14          |
| (1,875) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HB3  | 19       | 0.14          |
| (1,875) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HB3  | 19       | 0.14          |
| (1,875) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HB3  | 19       | 0.14          |
| (1,875) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HB3  | 19       | 0.14          |
| (1,870) | 1:17:A:VAL:HG11 | 1:57:A:ASN:H    | 16       | 0.14          |
| (1,870) | 1:17:A:VAL:HG12 | 1:57:A:ASN:H    | 16       | 0.14          |
| (1,870) | 1:17:A:VAL:HG13 | 1:57:A:ASN:H    | 16       | 0.14          |
| (1,870) | 1:17:A:VAL:HG21 | 1:57:A:ASN:H    | 16       | 0.14          |
| (1,870) | 1:17:A:VAL:HG22 | 1:57:A:ASN:H    | 16       | 0.14          |
| (1,870) | 1:17:A:VAL:HG23 | 1:57:A:ASN:H    | 16       | 0.14          |
| (1,867) | 1:17:A:VAL:HG11 | 1:55:A:CYS:CB   | 16       | 0.14          |
| (1,867) | 1:17:A:VAL:HG12 | 1:55:A:CYS:CB   | 16       | 0.14          |
| (1,867) | 1:17:A:VAL:HG13 | 1:55:A:CYS:CB   | 16       | 0.14          |
| (1,867) | 1:17:A:VAL:HG21 | 1:55:A:CYS:CB   | 16       | 0.14          |
| (1,867) | 1:17:A:VAL:HG22 | 1:55:A:CYS:CB   | 16       | 0.14          |
| (1,867) | 1:17:A:VAL:HG23 | 1:55:A:CYS:CB   | 16       | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 3        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 3        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 3        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 3        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 3        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 3        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 5        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 5        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 5        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 5        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 5        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 5        | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 17       | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 17       | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 17       | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 17       | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 17       | 0.14          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 17       | 0.14          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD11 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD12 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD13 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD21 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD22 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD23 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD11 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD12 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD13 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD21 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD22 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD23 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD11 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD12 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD13 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD21 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD22 | 16       | 0.14          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD23 | 16       | 0.14          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG21 | 16       | 0.14          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG22 | 16       | 0.14          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG23 | 16       | 0.14          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD11 | 17       | 0.14          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD12 | 17       | 0.14          |
| (1,726) | 1:22:A:VAL:CG1  | 1:46:A:ILE:HD13 | 17       | 0.14          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 10       | 0.14          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 14       | 0.14          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 14       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 14       | 0.14          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 14       | 0.14          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 14       | 0.14          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 14       | 0.14          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 14       | 0.14          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 14       | 0.14          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 14       | 0.14          |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD11 | 13       | 0.14          |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD12 | 13       | 0.14          |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD13 | 13       | 0.14          |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD11 | 13       | 0.14          |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD12 | 13       | 0.14          |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD13 | 13       | 0.14          |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD11 | 13       | 0.14          |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD12 | 13       | 0.14          |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD13 | 13       | 0.14          |
| (1,704) | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG11 | 9        | 0.14          |
| (1,704) | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG12 | 9        | 0.14          |
| (1,704) | 1:54:A:ILE:HG21 | 1:56:A:VAL:HG13 | 9        | 0.14          |
| (1,704) | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG11 | 9        | 0.14          |
| (1,704) | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG12 | 9        | 0.14          |
| (1,704) | 1:54:A:ILE:HG22 | 1:56:A:VAL:HG13 | 9        | 0.14          |
| (1,704) | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG11 | 9        | 0.14          |
| (1,704) | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG12 | 9        | 0.14          |
| (1,704) | 1:54:A:ILE:HG23 | 1:56:A:VAL:HG13 | 9        | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 4        | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 4        | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 4        | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 7        | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 7        | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 7        | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 18       | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 18       | 0.14          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 18       | 0.14          |
| (1,673) | 1:42:A:THR:HB   | 1:58:A:PRO:HG3  | 3        | 0.14          |
| (1,669) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HA   | 9        | 0.14          |
| (1,669) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HA   | 9        | 0.14          |
| (1,669) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HA   | 9        | 0.14          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD21 | 13       | 0.14          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD22 | 13       | 0.14          |
| (1,631) | 1:10:A:LEU:HA   | 1:10:A:LEU:HD23 | 13       | 0.14          |
| (1,612) | 1:65:A:ARG:HA   | 1:68:A:ARG:HB3  | 2        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,610) | 1:50:A:MET:HB3  | 1:50:A:MET:HE1  | 16       | 0.14          |
| (1,610) | 1:50:A:MET:HB3  | 1:50:A:MET:HE2  | 16       | 0.14          |
| (1,610) | 1:50:A:MET:HB3  | 1:50:A:MET:HE3  | 16       | 0.14          |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG21  | 5        | 0.14          |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG22  | 5        | 0.14          |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG23  | 5        | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 2        | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 2        | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 2        | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 4        | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 4        | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 4        | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 10       | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 10       | 0.14          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 10       | 0.14          |
| (1,329) | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 8        | 0.14          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD21 | 5        | 0.14          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD22 | 5        | 0.14          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD23 | 5        | 0.14          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD21 | 10       | 0.14          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD22 | 10       | 0.14          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD23 | 10       | 0.14          |
| (1,285) | 1:44:A:VAL:HG21 | 1:58:A:PRO:HB3  | 5        | 0.14          |
| (1,285) | 1:44:A:VAL:HG22 | 1:58:A:PRO:HB3  | 5        | 0.14          |
| (1,285) | 1:44:A:VAL:HG23 | 1:58:A:PRO:HB3  | 5        | 0.14          |
| (1,285) | 1:44:A:VAL:HG21 | 1:58:A:PRO:HB3  | 11       | 0.14          |
| (1,285) | 1:44:A:VAL:HG22 | 1:58:A:PRO:HB3  | 11       | 0.14          |
| (1,285) | 1:44:A:VAL:HG23 | 1:58:A:PRO:HB3  | 11       | 0.14          |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 16       | 0.14          |
| (1,263) | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 16       | 0.14          |
| (1,263) | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 16       | 0.14          |
| (1,256) | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB3  | 3        | 0.14          |
| (1,255) | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 8        | 0.14          |
| (1,252) | 1:57:A:ASN:HB2  | 1:57:A:ASN:HD22 | 1        | 0.14          |
| (1,249) | 1:48:A:THR:HG1  | 1:52:A:LYS:H    | 16       | 0.14          |
| (1,239) | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 13       | 0.14          |
| (1,239) | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 13       | 0.14          |
| (1,239) | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 13       | 0.14          |
| (1,147) | 1:49:A:LYS:H    | 1:49:A:LYS:HG2  | 3        | 0.14          |
| (1,66)  | 1:18:A:ILE:HG21 | 1:20:A:THR:H    | 8        | 0.14          |
| (1,66)  | 1:18:A:ILE:HG22 | 1:20:A:THR:H    | 8        | 0.14          |
| (1,66)  | 1:18:A:ILE:HG23 | 1:20:A:THR:H    | 8        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2)    | 1:13:A:ARG:H    | 1:14:A:CYS:H    | 1        | 0.14          |
| (3,27)   | 1:48:A:THR:H    | 1:52:A:LYS:O    | 17       | 0.13          |
| (1,1077) | 1:68:A:ARG:HA   | 1:71:A:GLN:HE21 | 11       | 0.13          |
| (1,1077) | 1:68:A:ARG:HA   | 1:71:A:GLN:HE22 | 11       | 0.13          |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB2  | 8        | 0.13          |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB3  | 8        | 0.13          |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB2  | 8        | 0.13          |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB3  | 8        | 0.13          |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB2  | 8        | 0.13          |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB3  | 8        | 0.13          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD11 | 16       | 0.13          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD12 | 16       | 0.13          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD13 | 16       | 0.13          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD21 | 16       | 0.13          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD22 | 16       | 0.13          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD23 | 16       | 0.13          |
| (1,1004) | 1:51:A:LYS:H    | 1:52:A:LYS:HD2  | 4        | 0.13          |
| (1,1004) | 1:51:A:LYS:H    | 1:52:A:LYS:HD3  | 4        | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG11 | 9        | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG12 | 9        | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG13 | 9        | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 9        | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 9        | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 9        | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG11 | 11       | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG12 | 11       | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG13 | 11       | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 11       | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 11       | 0.13          |
| (1,992)  | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 11       | 0.13          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 4        | 0.13          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 4        | 0.13          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 13       | 0.13          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 13       | 0.13          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 9        | 0.13          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 9        | 0.13          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 9        | 0.13          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 9        | 0.13          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 12       | 0.13          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 12       | 0.13          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 12       | 0.13          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 12       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD11 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD12 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD13 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD21 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD22 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD23 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD11 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD12 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD13 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD21 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD22 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD23 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD11 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD12 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD13 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD21 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD22 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD23 | 6        | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD11 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD12 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD13 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD21 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD22 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD23 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD11 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD12 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD13 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD21 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD22 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD23 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD11 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD12 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD13 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD21 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD22 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD23 | 14       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD11 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD12 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD13 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD21 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD22 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD23 | 19       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD11 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD12 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD13 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD21 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD22 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD23 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD11 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD12 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD13 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD21 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD22 | 19       | 0.13          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD23 | 19       | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 1        | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 1        | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 1        | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 1        | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 1        | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 1        | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 10       | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 10       | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 10       | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 10       | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 10       | 0.13          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 10       | 0.13          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 7        | 0.13          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 7        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,899) | 1:22:A:VAL:HG11 | 1:48:A:THR:HG21 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG11 | 1:48:A:THR:HG22 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG11 | 1:48:A:THR:HG23 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG12 | 1:48:A:THR:HG21 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG12 | 1:48:A:THR:HG22 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG12 | 1:48:A:THR:HG23 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG13 | 1:48:A:THR:HG21 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG13 | 1:48:A:THR:HG22 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG13 | 1:48:A:THR:HG23 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG21 | 1:48:A:THR:HG21 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG21 | 1:48:A:THR:HG22 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG21 | 1:48:A:THR:HG23 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG22 | 1:48:A:THR:HG21 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG22 | 1:48:A:THR:HG22 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG22 | 1:48:A:THR:HG23 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG23 | 1:48:A:THR:HG21 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG23 | 1:48:A:THR:HG22 | 6        | 0.13          |
| (1,899) | 1:22:A:VAL:HG23 | 1:48:A:THR:HG23 | 6        | 0.13          |
| (1,854) | 1:13:A:ARG:H    | 1:13:A:ARG:HG2  | 3        | 0.13          |
| (1,854) | 1:13:A:ARG:H    | 1:13:A:ARG:HG3  | 3        | 0.13          |
| (1,847) | 1:10:A:LEU:HD11 | 1:11:A:LYS:H    | 3        | 0.13          |
| (1,847) | 1:10:A:LEU:HD12 | 1:11:A:LYS:H    | 3        | 0.13          |
| (1,847) | 1:10:A:LEU:HD13 | 1:11:A:LYS:H    | 3        | 0.13          |
| (1,847) | 1:10:A:LEU:HD21 | 1:11:A:LYS:H    | 3        | 0.13          |
| (1,847) | 1:10:A:LEU:HD22 | 1:11:A:LYS:H    | 3        | 0.13          |
| (1,847) | 1:10:A:LEU:HD23 | 1:11:A:LYS:H    | 3        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 2        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 2        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 2        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 2        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 2        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 2        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 9        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 9        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 9        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 9        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 9        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 9        | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 10       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 10       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 10       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 10       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 10       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 10       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 11       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 11       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 11       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 11       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 11       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 11       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 12       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 12       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 12       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 12       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 12       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 12       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 20       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 20       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 20       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 20       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 20       | 0.13          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 20       | 0.13          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG21 | 3        | 0.13          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG22 | 3        | 0.13          |
| (1,803) | 1:22:A:VAL:CG2  | 1:26:A:ILE:HG23 | 3        | 0.13          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 5        | 0.13          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 7        | 0.13          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 7        | 0.13          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 7        | 0.13          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 7        | 0.13          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 7        | 0.13          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 7        | 0.13          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 7        | 0.13          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 7        | 0.13          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 7        | 0.13          |
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD21 | 10       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD22 | 10       | 0.13          |
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD23 | 10       | 0.13          |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD21 | 10       | 0.13          |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD22 | 10       | 0.13          |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD23 | 10       | 0.13          |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD21 | 10       | 0.13          |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD22 | 10       | 0.13          |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD23 | 10       | 0.13          |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD11 | 12       | 0.13          |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD12 | 12       | 0.13          |
| (1,706) | 1:56:A:VAL:HG21 | 1:63:A:LEU:HD13 | 12       | 0.13          |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD11 | 12       | 0.13          |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD12 | 12       | 0.13          |
| (1,706) | 1:56:A:VAL:HG22 | 1:63:A:LEU:HD13 | 12       | 0.13          |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD11 | 12       | 0.13          |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD12 | 12       | 0.13          |
| (1,706) | 1:56:A:VAL:HG23 | 1:63:A:LEU:HD13 | 12       | 0.13          |
| (1,705) | 1:42:A:THR:HG21 | 1:58:A:PRO:HG3  | 6        | 0.13          |
| (1,705) | 1:42:A:THR:HG22 | 1:58:A:PRO:HG3  | 6        | 0.13          |
| (1,705) | 1:42:A:THR:HG23 | 1:58:A:PRO:HG3  | 6        | 0.13          |
| (1,705) | 1:42:A:THR:HG21 | 1:58:A:PRO:HG3  | 17       | 0.13          |
| (1,705) | 1:42:A:THR:HG22 | 1:58:A:PRO:HG3  | 17       | 0.13          |
| (1,705) | 1:42:A:THR:HG23 | 1:58:A:PRO:HG3  | 17       | 0.13          |
| (1,705) | 1:42:A:THR:HG21 | 1:58:A:PRO:HG3  | 20       | 0.13          |
| (1,705) | 1:42:A:THR:HG22 | 1:58:A:PRO:HG3  | 20       | 0.13          |
| (1,705) | 1:42:A:THR:HG23 | 1:58:A:PRO:HG3  | 20       | 0.13          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 9        | 0.13          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 9        | 0.13          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 9        | 0.13          |
| (1,674) | 1:39:A:CYS:HA   | 1:40:A:PRO:HD2  | 4        | 0.13          |
| (1,667) | 1:17:A:VAL:HB   | 1:57:A:ASN:HA   | 7        | 0.13          |
| (1,586) | 1:27:A:ILE:HD11 | 1:62:A:TRP:HZ3  | 7        | 0.13          |
| (1,586) | 1:27:A:ILE:HD12 | 1:62:A:TRP:HZ3  | 7        | 0.13          |
| (1,586) | 1:27:A:ILE:HD13 | 1:62:A:TRP:HZ3  | 7        | 0.13          |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG21  | 6        | 0.13          |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG22  | 6        | 0.13          |
| (1,580) | 1:8:A:THR:H     | 1:8:A:THR:HG23  | 6        | 0.13          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG21 | 1        | 0.13          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG22 | 1        | 0.13          |
| (1,497) | 1:47:A:TRP:HE1  | 1:53:A:VAL:HG23 | 1        | 0.13          |
| (1,477) | 1:30:A:ILE:H    | 1:30:A:ILE:HD11 | 3        | 0.13          |
| (1,477) | 1:30:A:ILE:H    | 1:30:A:ILE:HD12 | 3        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,477)  | 1:30:A:ILE:H    | 1:30:A:ILE:HD13 | 3        | 0.13          |
| (1,459)  | 1:13:A:ARG:H    | 1:13:A:ARG:HG2  | 3        | 0.13          |
| (1,454)  | 1:11:A:LYS:H    | 1:11:A:LYS:HG3  | 11       | 0.13          |
| (1,329)  | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 19       | 0.13          |
| (1,328)  | 1:57:A:ASN:HA   | 1:58:A:PRO:HD3  | 13       | 0.13          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD11 | 10       | 0.13          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD12 | 10       | 0.13          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD13 | 10       | 0.13          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD11 | 12       | 0.13          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD12 | 12       | 0.13          |
| (1,290)  | 1:66:A:LEU:HA   | 1:66:A:LEU:HD13 | 12       | 0.13          |
| (1,263)  | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 1        | 0.13          |
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 1        | 0.13          |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 1        | 0.13          |
| (1,263)  | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 2        | 0.13          |
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 2        | 0.13          |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 2        | 0.13          |
| (1,263)  | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 19       | 0.13          |
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 19       | 0.13          |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 19       | 0.13          |
| (1,263)  | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 20       | 0.13          |
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 20       | 0.13          |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 20       | 0.13          |
| (1,255)  | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 4        | 0.13          |
| (1,255)  | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 5        | 0.13          |
| (1,255)  | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB2  | 16       | 0.13          |
| (1,205)  | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 17       | 0.13          |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG11 | 7        | 0.13          |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG12 | 7        | 0.13          |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG13 | 7        | 0.13          |
| (3,27)   | 1:48:A:THR:H    | 1:52:A:LYS:O    | 19       | 0.12          |
| (3,19)   | 1:33:A:THR:O    | 1:43:A:GLU:H    | 7        | 0.12          |
| (3,15)   | 1:4:A:GLU:O     | 1:32:A:VAL:H    | 15       | 0.12          |
| (1,1087) | 1:75:A:LEU:HA   | 1:75:A:LEU:HD11 | 5        | 0.12          |
| (1,1087) | 1:75:A:LEU:HA   | 1:75:A:LEU:HD12 | 5        | 0.12          |
| (1,1087) | 1:75:A:LEU:HA   | 1:75:A:LEU:HD13 | 5        | 0.12          |
| (1,1087) | 1:75:A:LEU:HA   | 1:75:A:LEU:HD21 | 5        | 0.12          |
| (1,1087) | 1:75:A:LEU:HA   | 1:75:A:LEU:HD22 | 5        | 0.12          |
| (1,1087) | 1:75:A:LEU:HA   | 1:75:A:LEU:HD23 | 5        | 0.12          |
| (1,1082) | 1:70:A:VAL:HG11 | 1:71:A:GLN:H    | 17       | 0.12          |
| (1,1082) | 1:70:A:VAL:HG12 | 1:71:A:GLN:H    | 17       | 0.12          |
| (1,1082) | 1:70:A:VAL:HG13 | 1:71:A:GLN:H    | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1082) | 1:70:A:VAL:HG21 | 1:71:A:GLN:H    | 17       | 0.12          |
| (1,1082) | 1:70:A:VAL:HG22 | 1:71:A:GLN:H    | 17       | 0.12          |
| (1,1082) | 1:70:A:VAL:HG23 | 1:71:A:GLN:H    | 17       | 0.12          |
| (1,1077) | 1:68:A:ARG:HA   | 1:71:A:GLN:HE21 | 20       | 0.12          |
| (1,1077) | 1:68:A:ARG:HA   | 1:71:A:GLN:HE22 | 20       | 0.12          |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB2  | 10       | 0.12          |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB3  | 10       | 0.12          |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB2  | 10       | 0.12          |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB3  | 10       | 0.12          |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB2  | 10       | 0.12          |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB3  | 10       | 0.12          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD11 | 18       | 0.12          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD12 | 18       | 0.12          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD13 | 18       | 0.12          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD21 | 18       | 0.12          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD22 | 18       | 0.12          |
| (1,1038) | 1:63:A:LEU:HA   | 1:66:A:LEU:HD23 | 18       | 0.12          |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG11 | 8        | 0.12          |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG12 | 8        | 0.12          |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG13 | 8        | 0.12          |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG21 | 8        | 0.12          |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG22 | 8        | 0.12          |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG23 | 8        | 0.12          |
| (1,969)  | 1:39:A:CYS:HA   | 1:40:A:PRO:HD2  | 10       | 0.12          |
| (1,969)  | 1:39:A:CYS:HA   | 1:40:A:PRO:HD3  | 10       | 0.12          |
| (1,969)  | 1:39:A:CYS:HA   | 1:40:A:PRO:HD2  | 17       | 0.12          |
| (1,969)  | 1:39:A:CYS:HA   | 1:40:A:PRO:HD3  | 17       | 0.12          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 11       | 0.12          |
| (1,963)  | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 11       | 0.12          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 1        | 0.12          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 1        | 0.12          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 1        | 0.12          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 1        | 0.12          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 5        | 0.12          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 5        | 0.12          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 5        | 0.12          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 5        | 0.12          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 19       | 0.12          |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 19       | 0.12          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 19       | 0.12          |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 19       | 0.12          |
| (1,921)  | 1:26:A:ILE:HA   | 1:49:A:LYS:HG2  | 10       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,921) | 1:26:A:ILE:HA   | 1:49:A:LYS:HG3  | 10       | 0.12          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 17       | 0.12          |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 17       | 0.12          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 7        | 0.12          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 7        | 0.12          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 7        | 0.12          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 7        | 0.12          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 7        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 7        | 0.12          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 15       | 0.12          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 15       | 0.12          |
| (1,884) | 1:21:A:VAL:HG11 | 1:62:A:TRP:HB2  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG11 | 1:62:A:TRP:HB3  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG12 | 1:62:A:TRP:HB2  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG12 | 1:62:A:TRP:HB3  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG13 | 1:62:A:TRP:HB2  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG13 | 1:62:A:TRP:HB3  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG21 | 1:62:A:TRP:HB2  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG21 | 1:62:A:TRP:HB3  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG22 | 1:62:A:TRP:HB2  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG22 | 1:62:A:TRP:HB3  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG23 | 1:62:A:TRP:HB2  | 2        | 0.12          |
| (1,884) | 1:21:A:VAL:HG23 | 1:62:A:TRP:HB3  | 2        | 0.12          |
| (1,875) | 1:17:A:VAL:HG11 | 1:57:A:ASN:HB3  | 20       | 0.12          |
| (1,875) | 1:17:A:VAL:HG12 | 1:57:A:ASN:HB3  | 20       | 0.12          |
| (1,875) | 1:17:A:VAL:HG13 | 1:57:A:ASN:HB3  | 20       | 0.12          |
| (1,875) | 1:17:A:VAL:HG21 | 1:57:A:ASN:HB3  | 20       | 0.12          |
| (1,875) | 1:17:A:VAL:HG22 | 1:57:A:ASN:HB3  | 20       | 0.12          |
| (1,875) | 1:17:A:VAL:HG23 | 1:57:A:ASN:HB3  | 20       | 0.12          |
| (1,860) | 1:14:A:CYS:HB2  | 1:45:A:VAL:HG21 | 5        | 0.12          |
| (1,860) | 1:14:A:CYS:HB2  | 1:45:A:VAL:HG22 | 5        | 0.12          |
| (1,860) | 1:14:A:CYS:HB2  | 1:45:A:VAL:HG23 | 5        | 0.12          |
| (1,860) | 1:14:A:CYS:HB3  | 1:45:A:VAL:HG21 | 5        | 0.12          |
| (1,860) | 1:14:A:CYS:HB3  | 1:45:A:VAL:HG22 | 5        | 0.12          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,860) | 1:14:A:CYS:HB3 | 1:45:A:VAL:HG23 | 5        | 0.12          |
| (1,852) | 1:12:A:CYS:HB2 | 1:14:A:CYS:H    | 13       | 0.12          |
| (1,852) | 1:12:A:CYS:HB3 | 1:14:A:CYS:H    | 13       | 0.12          |
| (1,846) | 1:10:A:LEU:HB2 | 1:11:A:LYS:H    | 15       | 0.12          |
| (1,846) | 1:10:A:LEU:HB3 | 1:11:A:LYS:H    | 15       | 0.12          |
| (1,824) | 1:3:A:LEU:HD11 | 1:67:A:LEU:HD21 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD11 | 1:67:A:LEU:HD22 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD11 | 1:67:A:LEU:HD23 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD12 | 1:67:A:LEU:HD21 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD12 | 1:67:A:LEU:HD22 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD12 | 1:67:A:LEU:HD23 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD13 | 1:67:A:LEU:HD21 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD13 | 1:67:A:LEU:HD22 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD13 | 1:67:A:LEU:HD23 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD21 | 1:67:A:LEU:HD21 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD21 | 1:67:A:LEU:HD22 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD21 | 1:67:A:LEU:HD23 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD22 | 1:67:A:LEU:HD21 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD22 | 1:67:A:LEU:HD22 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD22 | 1:67:A:LEU:HD23 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD23 | 1:67:A:LEU:HD21 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD23 | 1:67:A:LEU:HD22 | 14       | 0.12          |
| (1,824) | 1:3:A:LEU:HD23 | 1:67:A:LEU:HD23 | 14       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD11  | 13       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD12  | 13       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD13  | 13       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD21  | 13       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD22  | 13       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD23  | 13       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD11  | 15       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD12  | 15       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD13  | 15       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD21  | 15       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD22  | 15       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD23  | 15       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD11  | 16       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD12  | 16       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD13  | 16       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD21  | 16       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD22  | 16       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD23  | 16       | 0.12          |
| (1,818) | 1:3:A:LEU:HA   | 1:3:A:LEU:HD11  | 19       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 19       | 0.12          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 19       | 0.12          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 19       | 0.12          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 19       | 0.12          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 19       | 0.12          |
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD21 | 2        | 0.12          |
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD22 | 2        | 0.12          |
| (1,708) | 1:44:A:VAL:HG11 | 1:63:A:LEU:HD23 | 2        | 0.12          |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD21 | 2        | 0.12          |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD22 | 2        | 0.12          |
| (1,708) | 1:44:A:VAL:HG12 | 1:63:A:LEU:HD23 | 2        | 0.12          |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD21 | 2        | 0.12          |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD22 | 2        | 0.12          |
| (1,708) | 1:44:A:VAL:HG13 | 1:63:A:LEU:HD23 | 2        | 0.12          |
| (1,705) | 1:42:A:THR:HG21 | 1:58:A:PRO:HG3  | 10       | 0.12          |
| (1,705) | 1:42:A:THR:HG22 | 1:58:A:PRO:HG3  | 10       | 0.12          |
| (1,705) | 1:42:A:THR:HG23 | 1:58:A:PRO:HG3  | 10       | 0.12          |
| (1,705) | 1:42:A:THR:HG21 | 1:58:A:PRO:HG3  | 14       | 0.12          |
| (1,705) | 1:42:A:THR:HG22 | 1:58:A:PRO:HG3  | 14       | 0.12          |
| (1,705) | 1:42:A:THR:HG23 | 1:58:A:PRO:HG3  | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD21 | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD22 | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD23 | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD21 | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD22 | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD23 | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD21 | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD22 | 14       | 0.12          |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD23 | 14       | 0.12          |
| (1,678) | 1:44:A:VAL:HG21 | 1:63:A:LEU:HD21 | 16       | 0.12          |
| (1,678) | 1:44:A:VAL:HG21 | 1:63:A:LEU:HD22 | 16       | 0.12          |
| (1,678) | 1:44:A:VAL:HG21 | 1:63:A:LEU:HD23 | 16       | 0.12          |
| (1,678) | 1:44:A:VAL:HG22 | 1:63:A:LEU:HD21 | 16       | 0.12          |
| (1,678) | 1:44:A:VAL:HG22 | 1:63:A:LEU:HD22 | 16       | 0.12          |
| (1,678) | 1:44:A:VAL:HG22 | 1:63:A:LEU:HD23 | 16       | 0.12          |
| (1,678) | 1:44:A:VAL:HG23 | 1:63:A:LEU:HD21 | 16       | 0.12          |
| (1,678) | 1:44:A:VAL:HG23 | 1:63:A:LEU:HD22 | 16       | 0.12          |
| (1,678) | 1:44:A:VAL:HG23 | 1:63:A:LEU:HD23 | 16       | 0.12          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 8        | 0.12          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 8        | 0.12          |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 8        | 0.12          |
| (1,586) | 1:27:A:ILE:HD11 | 1:62:A:TRP:HZ3  | 18       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,586) | 1:27:A:ILE:HD12 | 1:62:A:TRP:HZ3  | 18       | 0.12          |
| (1,586) | 1:27:A:ILE:HD13 | 1:62:A:TRP:HZ3  | 18       | 0.12          |
| (1,557) | 1:62:A:TRP:H    | 1:62:A:TRP:HD1  | 18       | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 5        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 5        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 5        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 6        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 6        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 6        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 7        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 7        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 7        | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 11       | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 11       | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 11       | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 16       | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 16       | 0.12          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 16       | 0.12          |
| (1,329) | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 13       | 0.12          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD21 | 17       | 0.12          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD22 | 17       | 0.12          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD23 | 17       | 0.12          |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 13       | 0.12          |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD22 | 13       | 0.12          |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD23 | 13       | 0.12          |
| (1,289) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD11 | 5        | 0.12          |
| (1,289) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD12 | 5        | 0.12          |
| (1,289) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD13 | 5        | 0.12          |
| (1,281) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HA   | 18       | 0.12          |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 4        | 0.12          |
| (1,263) | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 4        | 0.12          |
| (1,263) | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 4        | 0.12          |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 10       | 0.12          |
| (1,263) | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 10       | 0.12          |
| (1,263) | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 10       | 0.12          |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 11       | 0.12          |
| (1,263) | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 11       | 0.12          |
| (1,263) | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 11       | 0.12          |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 15       | 0.12          |
| (1,263) | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 15       | 0.12          |
| (1,263) | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 15       | 0.12          |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,263)  | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 17       | 0.12          |
| (1,263)  | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 17       | 0.12          |
| (1,239)  | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 3        | 0.12          |
| (1,239)  | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 3        | 0.12          |
| (1,239)  | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 3        | 0.12          |
| (1,215)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD11 | 6        | 0.12          |
| (1,215)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD12 | 6        | 0.12          |
| (1,215)  | 1:66:A:LEU:H    | 1:66:A:LEU:HD13 | 6        | 0.12          |
| (1,205)  | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 2        | 0.12          |
| (1,205)  | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 15       | 0.12          |
| (1,122)  | 1:40:A:PRO:HG2  | 1:41:A:LYS:H    | 7        | 0.12          |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG11 | 18       | 0.12          |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG12 | 18       | 0.12          |
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG13 | 18       | 0.12          |
| (3,35)   | 1:64:A:GLN:O    | 1:68:A:ARG:H    | 20       | 0.11          |
| (3,27)   | 1:48:A:THR:H    | 1:52:A:LYS:O    | 11       | 0.11          |
| (3,15)   | 1:4:A:GLU:O     | 1:32:A:VAL:H    | 6        | 0.11          |
| (1,1082) | 1:70:A:VAL:HG11 | 1:71:A:GLN:H    | 9        | 0.11          |
| (1,1082) | 1:70:A:VAL:HG12 | 1:71:A:GLN:H    | 9        | 0.11          |
| (1,1082) | 1:70:A:VAL:HG13 | 1:71:A:GLN:H    | 9        | 0.11          |
| (1,1082) | 1:70:A:VAL:HG21 | 1:71:A:GLN:H    | 9        | 0.11          |
| (1,1082) | 1:70:A:VAL:HG22 | 1:71:A:GLN:H    | 9        | 0.11          |
| (1,1082) | 1:70:A:VAL:HG23 | 1:71:A:GLN:H    | 9        | 0.11          |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB2  | 9        | 0.11          |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB3  | 9        | 0.11          |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB2  | 9        | 0.11          |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB3  | 9        | 0.11          |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB2  | 9        | 0.11          |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB3  | 9        | 0.11          |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB2  | 18       | 0.11          |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB3  | 18       | 0.11          |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB2  | 18       | 0.11          |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB3  | 18       | 0.11          |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB2  | 18       | 0.11          |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB3  | 18       | 0.11          |
| (1,1034) | 1:62:A:TRP:HE3  | 1:66:A:LEU:HD11 | 15       | 0.11          |
| (1,1034) | 1:62:A:TRP:HE3  | 1:66:A:LEU:HD12 | 15       | 0.11          |
| (1,1034) | 1:62:A:TRP:HE3  | 1:66:A:LEU:HD13 | 15       | 0.11          |
| (1,1034) | 1:62:A:TRP:HE3  | 1:66:A:LEU:HD21 | 15       | 0.11          |
| (1,1034) | 1:62:A:TRP:HE3  | 1:66:A:LEU:HD22 | 15       | 0.11          |
| (1,1034) | 1:62:A:TRP:HE3  | 1:66:A:LEU:HD23 | 15       | 0.11          |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG11 | 2        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,991) | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG12 | 2        | 0.11          |
| (1,991) | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG13 | 2        | 0.11          |
| (1,991) | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG21 | 2        | 0.11          |
| (1,991) | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG22 | 2        | 0.11          |
| (1,991) | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG23 | 2        | 0.11          |
| (1,969) | 1:39:A:CYS:HA   | 1:40:A:PRO:HD2  | 12       | 0.11          |
| (1,969) | 1:39:A:CYS:HA   | 1:40:A:PRO:HD3  | 12       | 0.11          |
| (1,969) | 1:39:A:CYS:HA   | 1:40:A:PRO:HD2  | 16       | 0.11          |
| (1,969) | 1:39:A:CYS:HA   | 1:40:A:PRO:HD3  | 16       | 0.11          |
| (1,969) | 1:39:A:CYS:HA   | 1:40:A:PRO:HD2  | 20       | 0.11          |
| (1,969) | 1:39:A:CYS:HA   | 1:40:A:PRO:HD3  | 20       | 0.11          |
| (1,963) | 1:33:A:THR:HA   | 1:34:A:PRO:HD2  | 18       | 0.11          |
| (1,963) | 1:33:A:THR:HA   | 1:34:A:PRO:HD3  | 18       | 0.11          |
| (1,932) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 13       | 0.11          |
| (1,932) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 13       | 0.11          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 13       | 0.11          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 13       | 0.11          |
| (1,932) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 18       | 0.11          |
| (1,932) | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 18       | 0.11          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 18       | 0.11          |
| (1,932) | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD11 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD12 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD13 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD21 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD22 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD11 | 1:66:A:LEU:HD23 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD11 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD12 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD13 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD21 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD22 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD12 | 1:66:A:LEU:HD23 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD11 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD12 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD13 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD21 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD22 | 18       | 0.11          |
| (1,925) | 1:27:A:ILE:HD13 | 1:66:A:LEU:HD23 | 18       | 0.11          |
| (1,924) | 1:27:A:ILE:HG21 | 1:30:A:ILE:HG12 | 1        | 0.11          |
| (1,924) | 1:27:A:ILE:HG21 | 1:30:A:ILE:HG13 | 1        | 0.11          |
| (1,924) | 1:27:A:ILE:HG22 | 1:30:A:ILE:HG12 | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,924) | 1:27:A:ILE:HG22 | 1:30:A:ILE:HG13 | 1        | 0.11          |
| (1,924) | 1:27:A:ILE:HG23 | 1:30:A:ILE:HG12 | 1        | 0.11          |
| (1,924) | 1:27:A:ILE:HG23 | 1:30:A:ILE:HG13 | 1        | 0.11          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 14       | 0.11          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 14       | 0.11          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 14       | 0.11          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 14       | 0.11          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 14       | 0.11          |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 14       | 0.11          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 3        | 0.11          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD11 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD12 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG11 | 1:54:A:ILE:HD13 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD11 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD12 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG12 | 1:54:A:ILE:HD13 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD11 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD12 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG13 | 1:54:A:ILE:HD13 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD11 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD12 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG21 | 1:54:A:ILE:HD13 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD11 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD12 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG22 | 1:54:A:ILE:HD13 | 10       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD11 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD12 | 10       | 0.11          |
| (1,900) | 1:22:A:VAL:HG23 | 1:54:A:ILE:HD13 | 10       | 0.11          |
| (1,870) | 1:17:A:VAL:HG11 | 1:57:A:ASN:H    | 15       | 0.11          |
| (1,870) | 1:17:A:VAL:HG12 | 1:57:A:ASN:H    | 15       | 0.11          |
| (1,870) | 1:17:A:VAL:HG13 | 1:57:A:ASN:H    | 15       | 0.11          |
| (1,870) | 1:17:A:VAL:HG21 | 1:57:A:ASN:H    | 15       | 0.11          |
| (1,870) | 1:17:A:VAL:HG22 | 1:57:A:ASN:H    | 15       | 0.11          |
| (1,870) | 1:17:A:VAL:HG23 | 1:57:A:ASN:H    | 15       | 0.11          |
| (1,846) | 1:10:A:LEU:HB2  | 1:11:A:LYS:H    | 13       | 0.11          |
| (1,846) | 1:10:A:LEU:HB3  | 1:11:A:LYS:H    | 13       | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 7        | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 7        | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 7        | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 7        | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 7        | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 7        | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 18       | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 18       | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 18       | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 18       | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 18       | 0.11          |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 18       | 0.11          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD11 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD12 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD13 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD21 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD22 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE1   | 1:66:A:LEU:HD23 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD11 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD12 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD13 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD21 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD22 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE2   | 1:66:A:LEU:HD23 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD11 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD12 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD13 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD21 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD22 | 20       | 0.11          |
| (1,812) | 1:1:A:MET:HE3   | 1:66:A:LEU:HD23 | 20       | 0.11          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG21 | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG22 | 1        | 0.11          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG23 | 1        | 0.11          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG21 | 19       | 0.11          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG22 | 19       | 0.11          |
| (1,771) | 1:30:A:ILE:CD1  | 1:46:A:ILE:HG23 | 19       | 0.11          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 16       | 0.11          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 16       | 0.11          |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 16       | 0.11          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 16       | 0.11          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 16       | 0.11          |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 16       | 0.11          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 16       | 0.11          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 16       | 0.11          |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 16       | 0.11          |
| (1,712) | 1:27:A:ILE:HG12 | 1:46:A:ILE:HG21 | 9        | 0.11          |
| (1,712) | 1:27:A:ILE:HG12 | 1:46:A:ILE:HG22 | 9        | 0.11          |
| (1,712) | 1:27:A:ILE:HG12 | 1:46:A:ILE:HG23 | 9        | 0.11          |
| (1,675) | 1:39:A:CYS:HA   | 1:40:A:PRO:HD3  | 11       | 0.11          |
| (1,671) | 1:81:A:ALA:HA   | 1:82:A:PRO:HD3  | 15       | 0.11          |
| (1,661) | 1:66:A:LEU:HA   | 1:69:A:HIS:HB3  | 11       | 0.11          |
| (1,661) | 1:66:A:LEU:HA   | 1:69:A:HIS:HB3  | 16       | 0.11          |
| (1,660) | 1:7:A:TYR:HA    | 1:7:A:TYR:HD2   | 7        | 0.11          |
| (1,649) | 1:78:A:THR:HA   | 1:79:A:PRO:HD3  | 10       | 0.11          |
| (1,646) | 1:61:A:LYS:HA   | 1:61:A:LYS:HD3  | 13       | 0.11          |
| (1,646) | 1:61:A:LYS:HA   | 1:61:A:LYS:HD3  | 14       | 0.11          |
| (1,619) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD21 | 3        | 0.11          |
| (1,619) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD22 | 3        | 0.11          |
| (1,619) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD23 | 3        | 0.11          |
| (1,349) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD11 | 18       | 0.11          |
| (1,349) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD12 | 18       | 0.11          |
| (1,349) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD13 | 18       | 0.11          |
| (1,349) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD11 | 18       | 0.11          |
| (1,349) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD12 | 18       | 0.11          |
| (1,349) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD13 | 18       | 0.11          |
| (1,349) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD11 | 18       | 0.11          |
| (1,349) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD12 | 18       | 0.11          |
| (1,349) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD13 | 18       | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 1        | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 1        | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 1        | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 3        | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 3        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 3        | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 15       | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 15       | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 15       | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 19       | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 19       | 0.11          |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 19       | 0.11          |
| (1,329) | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 2        | 0.11          |
| (1,329) | 1:4:A:GLU:HB2   | 1:31:A:GLN:HA   | 14       | 0.11          |
| (1,325) | 1:28:A:ASP:HA   | 1:49:A:LYS:HA   | 11       | 0.11          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD21 | 3        | 0.11          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD22 | 3        | 0.11          |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD23 | 3        | 0.11          |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD21 | 17       | 0.11          |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD22 | 17       | 0.11          |
| (1,291) | 1:24:A:LEU:HA   | 1:24:A:LEU:HD23 | 17       | 0.11          |
| (1,289) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD11 | 4        | 0.11          |
| (1,289) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD12 | 4        | 0.11          |
| (1,289) | 1:62:A:TRP:HZ3  | 1:66:A:LEU:HD13 | 4        | 0.11          |
| (1,280) | 1:26:A:ILE:HB   | 1:48:A:THR:HB   | 12       | 0.11          |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 8        | 0.11          |
| (1,263) | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 8        | 0.11          |
| (1,263) | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 8        | 0.11          |
| (1,263) | 1:56:A:VAL:HG11 | 1:62:A:TRP:HZ2  | 14       | 0.11          |
| (1,263) | 1:56:A:VAL:HG12 | 1:62:A:TRP:HZ2  | 14       | 0.11          |
| (1,263) | 1:56:A:VAL:HG13 | 1:62:A:TRP:HZ2  | 14       | 0.11          |
| (1,256) | 1:57:A:ASN:HD22 | 1:59:A:ARG:HB3  | 2        | 0.11          |
| (1,252) | 1:57:A:ASN:HB2  | 1:57:A:ASN:HD22 | 8        | 0.11          |
| (1,252) | 1:57:A:ASN:HB2  | 1:57:A:ASN:HD22 | 12       | 0.11          |
| (1,239) | 1:45:A:VAL:HG21 | 1:47:A:TRP:HE1  | 9        | 0.11          |
| (1,239) | 1:45:A:VAL:HG22 | 1:47:A:TRP:HE1  | 9        | 0.11          |
| (1,239) | 1:45:A:VAL:HG23 | 1:47:A:TRP:HE1  | 9        | 0.11          |
| (1,216) | 1:66:A:LEU:H    | 1:66:A:LEU:HD21 | 20       | 0.11          |
| (1,216) | 1:66:A:LEU:H    | 1:66:A:LEU:HD22 | 20       | 0.11          |
| (1,216) | 1:66:A:LEU:H    | 1:66:A:LEU:HD23 | 20       | 0.11          |
| (1,215) | 1:66:A:LEU:H    | 1:66:A:LEU:HD11 | 14       | 0.11          |
| (1,215) | 1:66:A:LEU:H    | 1:66:A:LEU:HD12 | 14       | 0.11          |
| (1,215) | 1:66:A:LEU:H    | 1:66:A:LEU:HD13 | 14       | 0.11          |
| (1,205) | 1:64:A:GLN:H    | 1:64:A:GLN:HG3  | 12       | 0.11          |
| (1,154) | 1:50:A:MET:H    | 1:50:A:MET:HG3  | 14       | 0.11          |
| (1,72)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG11 | 16       | 0.11          |
| (1,72)  | 1:21:A:VAL:H    | 1:21:A:VAL:HG12 | 16       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,72)   | 1:21:A:VAL:H    | 1:21:A:VAL:HG13 | 16       | 0.11          |
| (1,66)   | 1:18:A:ILE:HG21 | 1:20:A:THR:H    | 2        | 0.11          |
| (1,66)   | 1:18:A:ILE:HG22 | 1:20:A:THR:H    | 2        | 0.11          |
| (1,66)   | 1:18:A:ILE:HG23 | 1:20:A:THR:H    | 2        | 0.11          |
| (1,66)   | 1:18:A:ILE:HG21 | 1:20:A:THR:H    | 11       | 0.11          |
| (1,66)   | 1:18:A:ILE:HG22 | 1:20:A:THR:H    | 11       | 0.11          |
| (1,66)   | 1:18:A:ILE:HG23 | 1:20:A:THR:H    | 11       | 0.11          |
| (1,2)    | 1:13:A:ARG:H    | 1:14:A:CYS:H    | 18       | 0.11          |
| (3,35)   | 1:64:A:GLN:O    | 1:68:A:ARG:H    | 19       | 0.1           |
| (3,27)   | 1:48:A:THR:H    | 1:52:A:LYS:O    | 18       | 0.1           |
| (3,19)   | 1:33:A:THR:O    | 1:43:A:GLU:H    | 1        | 0.1           |
| (3,19)   | 1:33:A:THR:O    | 1:43:A:GLU:H    | 10       | 0.1           |
| (3,11)   | 1:2:A:ILE:O     | 1:30:A:ILE:H    | 3        | 0.1           |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB2  | 7        | 0.1           |
| (1,1039) | 1:63:A:LEU:HD11 | 1:66:A:LEU:HB3  | 7        | 0.1           |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB2  | 7        | 0.1           |
| (1,1039) | 1:63:A:LEU:HD12 | 1:66:A:LEU:HB3  | 7        | 0.1           |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB2  | 7        | 0.1           |
| (1,1039) | 1:63:A:LEU:HD13 | 1:66:A:LEU:HB3  | 7        | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG11 | 3        | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG12 | 3        | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG13 | 3        | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG21 | 3        | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG22 | 3        | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG23 | 3        | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG11 | 15       | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG12 | 15       | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG13 | 15       | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG21 | 15       | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG22 | 15       | 0.1           |
| (1,991)  | 1:47:A:TRP:HD1  | 1:53:A:VAL:HG23 | 15       | 0.1           |
| (1,969)  | 1:39:A:CYS:HA   | 1:40:A:PRO:HD2  | 4        | 0.1           |
| (1,969)  | 1:39:A:CYS:HA   | 1:40:A:PRO:HD3  | 4        | 0.1           |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG2  | 15       | 0.1           |
| (1,932)  | 1:28:A:ASP:HB2  | 1:49:A:LYS:HG3  | 15       | 0.1           |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG2  | 15       | 0.1           |
| (1,932)  | 1:28:A:ASP:HB3  | 1:49:A:LYS:HG3  | 15       | 0.1           |
| (1,921)  | 1:26:A:ILE:HA   | 1:49:A:LYS:HG2  | 14       | 0.1           |
| (1,921)  | 1:26:A:ILE:HA   | 1:49:A:LYS:HG3  | 14       | 0.1           |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD11 | 16       | 0.1           |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD12 | 16       | 0.1           |
| (1,918)  | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD13 | 16       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD21 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD22 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD11 | 1:66:A:LEU:HD23 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD11 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD12 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD13 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD21 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD22 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD12 | 1:66:A:LEU:HD23 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD11 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD12 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD13 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD21 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD22 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD13 | 1:66:A:LEU:HD23 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD11 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD12 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD13 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD21 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD22 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD21 | 1:66:A:LEU:HD23 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD11 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD12 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD13 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD21 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD22 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD22 | 1:66:A:LEU:HD23 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD11 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD12 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD13 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD21 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD22 | 16       | 0.1           |
| (1,918) | 1:24:A:LEU:HD23 | 1:66:A:LEU:HD23 | 16       | 0.1           |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD11 | 3        | 0.1           |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD12 | 3        | 0.1           |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD13 | 3        | 0.1           |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD21 | 3        | 0.1           |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD22 | 3        | 0.1           |
| (1,909) | 1:24:A:LEU:H    | 1:24:A:LEU:HD23 | 3        | 0.1           |
| (1,843) | 1:10:A:LEU:H    | 1:10:A:LEU:HD11 | 17       | 0.1           |
| (1,843) | 1:10:A:LEU:H    | 1:10:A:LEU:HD12 | 17       | 0.1           |
| (1,843) | 1:10:A:LEU:H    | 1:10:A:LEU:HD13 | 17       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,843) | 1:10:A:LEU:H    | 1:10:A:LEU:HD21 | 17       | 0.1           |
| (1,843) | 1:10:A:LEU:H    | 1:10:A:LEU:HD22 | 17       | 0.1           |
| (1,843) | 1:10:A:LEU:H    | 1:10:A:LEU:HD23 | 17       | 0.1           |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD11  | 1        | 0.1           |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD12  | 1        | 0.1           |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD13  | 1        | 0.1           |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD21  | 1        | 0.1           |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD22  | 1        | 0.1           |
| (1,818) | 1:3:A:LEU:HA    | 1:3:A:LEU:HD23  | 1        | 0.1           |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD11 | 3        | 0.1           |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD12 | 3        | 0.1           |
| (1,714) | 1:46:A:ILE:HD11 | 1:63:A:LEU:HD13 | 3        | 0.1           |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD11 | 3        | 0.1           |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD12 | 3        | 0.1           |
| (1,714) | 1:46:A:ILE:HD12 | 1:63:A:LEU:HD13 | 3        | 0.1           |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD11 | 3        | 0.1           |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD12 | 3        | 0.1           |
| (1,714) | 1:46:A:ILE:HD13 | 1:63:A:LEU:HD13 | 3        | 0.1           |
| (1,705) | 1:42:A:THR:HG21 | 1:58:A:PRO:HG3  | 7        | 0.1           |
| (1,705) | 1:42:A:THR:HG22 | 1:58:A:PRO:HG3  | 7        | 0.1           |
| (1,705) | 1:42:A:THR:HG23 | 1:58:A:PRO:HG3  | 7        | 0.1           |
| (1,705) | 1:42:A:THR:HG21 | 1:58:A:PRO:HG3  | 11       | 0.1           |
| (1,705) | 1:42:A:THR:HG22 | 1:58:A:PRO:HG3  | 11       | 0.1           |
| (1,705) | 1:42:A:THR:HG23 | 1:58:A:PRO:HG3  | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD21 | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD22 | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD11 | 1:66:A:LEU:HD23 | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD21 | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD22 | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD12 | 1:66:A:LEU:HD23 | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD21 | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD22 | 11       | 0.1           |
| (1,699) | 1:30:A:ILE:HD13 | 1:66:A:LEU:HD23 | 11       | 0.1           |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD11 | 1        | 0.1           |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD12 | 1        | 0.1           |
| (1,676) | 1:22:A:VAL:HB   | 1:27:A:ILE:HD13 | 1        | 0.1           |
| (1,659) | 1:7:A:TYR:HA    | 1:7:A:TYR:HD1   | 15       | 0.1           |
| (1,649) | 1:78:A:THR:HA   | 1:79:A:PRO:HD3  | 5        | 0.1           |
| (1,645) | 1:61:A:LYS:HA   | 1:61:A:LYS:HD2  | 2        | 0.1           |
| (1,586) | 1:27:A:ILE:HD11 | 1:62:A:TRP:HZ3  | 2        | 0.1           |
| (1,586) | 1:27:A:ILE:HD12 | 1:62:A:TRP:HZ3  | 2        | 0.1           |
| (1,586) | 1:27:A:ILE:HD13 | 1:62:A:TRP:HZ3  | 2        | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,490) | 1:42:A:THR:HG21 | 1:44:A:VAL:H    | 18       | 0.1           |
| (1,490) | 1:42:A:THR:HG22 | 1:44:A:VAL:H    | 18       | 0.1           |
| (1,490) | 1:42:A:THR:HG23 | 1:44:A:VAL:H    | 18       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 13       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 13       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 13       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 14       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 14       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 14       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 17       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 17       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 17       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD21 | 20       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD22 | 20       | 0.1           |
| (1,343) | 1:63:A:LEU:HB3  | 1:63:A:LEU:HD23 | 20       | 0.1           |
| (1,323) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD21 | 18       | 0.1           |
| (1,323) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD22 | 18       | 0.1           |
| (1,323) | 1:67:A:LEU:HA   | 1:67:A:LEU:HD23 | 18       | 0.1           |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD21 | 2        | 0.1           |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD22 | 2        | 0.1           |
| (1,297) | 1:58:A:PRO:HA   | 1:63:A:LEU:HD23 | 2        | 0.1           |
| (1,296) | 1:44:A:VAL:HG21 | 1:58:A:PRO:HA   | 16       | 0.1           |
| (1,296) | 1:44:A:VAL:HG22 | 1:58:A:PRO:HA   | 16       | 0.1           |
| (1,296) | 1:44:A:VAL:HG23 | 1:58:A:PRO:HA   | 16       | 0.1           |
| (1,252) | 1:57:A:ASN:HB2  | 1:57:A:ASN:HD22 | 3        | 0.1           |
| (1,147) | 1:49:A:LYS:H    | 1:49:A:LYS:HG2  | 2        | 0.1           |
| (1,67)  | 1:18:A:ILE:HD11 | 1:20:A:THR:H    | 10       | 0.1           |
| (1,67)  | 1:18:A:ILE:HD12 | 1:20:A:THR:H    | 10       | 0.1           |
| (1,67)  | 1:18:A:ILE:HD13 | 1:20:A:THR:H    | 10       | 0.1           |

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

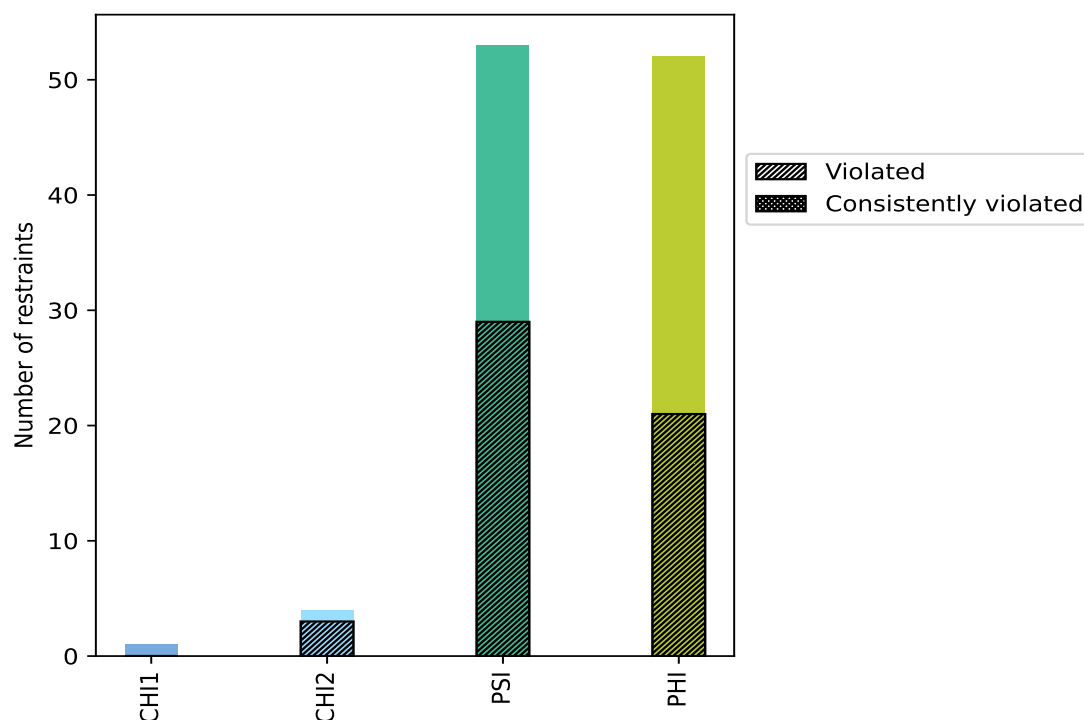
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| CHI1       | 1     | 0.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| CHI2       | 4     | 3.6            | 3                     | 75.0           | 2.7            | 0                                  | 0.0            | 0.0            |
| PSI        | 53    | 48.2           | 29                    | 54.7           | 26.4           | 0                                  | 0.0            | 0.0            |
| PHI        | 52    | 47.3           | 21                    | 40.4           | 19.1           | 0                                  | 0.0            | 0.0            |
| Total      | 110   | 100.0          | 53                    | 48.2           | 48.2           | 0                                  | 0.0            | 0.0            |

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

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



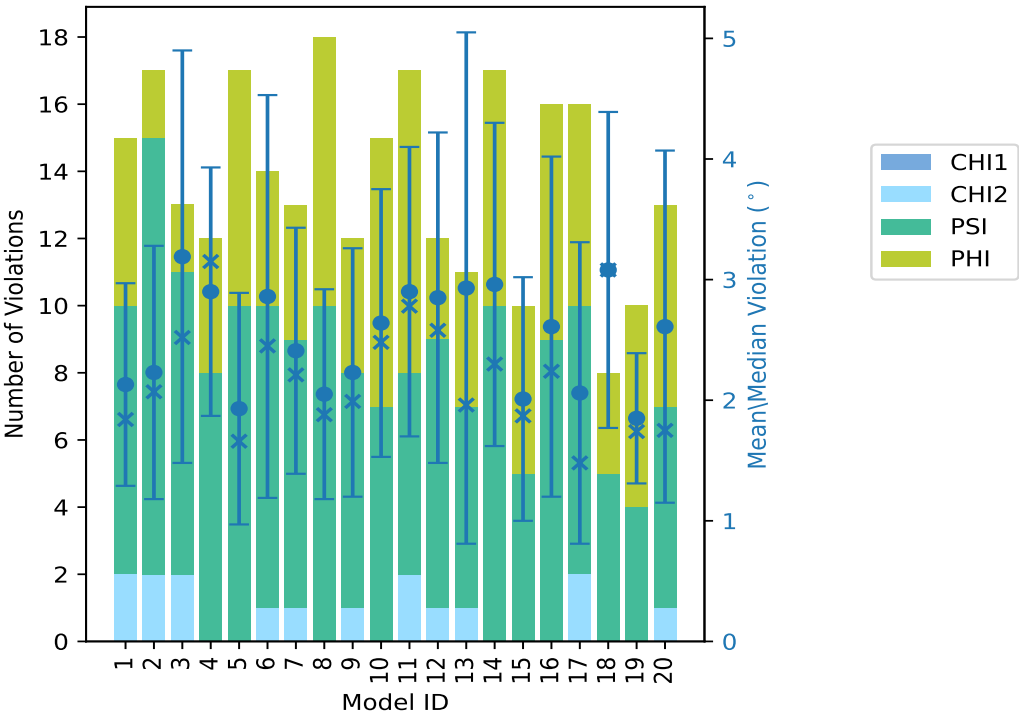
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations |      |     |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|------|-----|-----|-------|----------|---------|--------|------------|
|          | CHI1                 | CHI2 | PSI | PHI | Total |          |         |        |            |
| 1        | 0                    | 2    | 8   | 5   | 15    | 2.13     | 4.24    | 0.84   | 1.84       |
| 2        | 0                    | 2    | 13  | 2   | 17    | 2.23     | 5.1     | 1.05   | 2.07       |
| 3        | 0                    | 2    | 9   | 2   | 13    | 3.19     | 7.74    | 1.71   | 2.52       |
| 4        | 0                    | 0    | 8   | 4   | 12    | 2.9      | 4.57    | 1.03   | 3.15       |
| 5        | 0                    | 0    | 10  | 7   | 17    | 1.93     | 4.79    | 0.96   | 1.66       |
| 6        | 0                    | 1    | 9   | 4   | 14    | 2.86     | 7.04    | 1.67   | 2.45       |
| 7        | 0                    | 1    | 8   | 4   | 13    | 2.41     | 5.51    | 1.02   | 2.21       |
| 8        | 0                    | 0    | 10  | 8   | 18    | 2.05     | 4.21    | 0.87   | 1.88       |
| 9        | 0                    | 1    | 7   | 4   | 12    | 2.23     | 4.14    | 1.03   | 1.99       |
| 10       | 0                    | 0    | 7   | 8   | 15    | 2.64     | 4.61    | 1.11   | 2.48       |
| 11       | 0                    | 2    | 6   | 9   | 17    | 2.9      | 5.21    | 1.2    | 2.78       |
| 12       | 0                    | 1    | 8   | 3   | 12    | 2.85     | 5.21    | 1.37   | 2.58       |
| 13       | 0                    | 1    | 6   | 4   | 11    | 2.93     | 8.31    | 2.12   | 1.96       |
| 14       | 0                    | 0    | 10  | 7   | 17    | 2.96     | 5.68    | 1.34   | 2.3        |
| 15       | 0                    | 0    | 5   | 5   | 10    | 2.01     | 4.79    | 1.01   | 1.87       |
| 16       | 0                    | 0    | 9   | 7   | 16    | 2.61     | 6.55    | 1.41   | 2.24       |
| 17       | 0                    | 2    | 8   | 6   | 16    | 2.06     | 5.87    | 1.25   | 1.48       |
| 18       | 0                    | 0    | 5   | 3   | 8     | 3.08     | 4.77    | 1.31   | 3.08       |
| 19       | 0                    | 0    | 4   | 6   | 10    | 1.85     | 2.95    | 0.54   | 1.74       |
| 20       | 0                    | 1    | 6   | 6   | 13    | 2.61     | 5.94    | 1.46   | 1.75       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

| Number of violated restraints |      |     |     |       | Fraction of the ensemble |      |
|-------------------------------|------|-----|-----|-------|--------------------------|------|
| CHI1                          | CHI2 | PSI | PHI | Total | Count <sup>1</sup>       | %    |
| 0                             | 1    | 5   | 3   | 9     | 1                        | 5.0  |
| 0                             | 0    | 7   | 2   | 9     | 2                        | 10.0 |
| 0                             | 0    | 3   | 5   | 8     | 3                        | 15.0 |
| 0                             | 0    | 1   | 1   | 2     | 4                        | 20.0 |
| 0                             | 0    | 0   | 3   | 3     | 5                        | 25.0 |
| 0                             | 1    | 2   | 1   | 4     | 6                        | 30.0 |
| 0                             | 0    | 1   | 2   | 3     | 7                        | 35.0 |
| 0                             | 0    | 4   | 2   | 6     | 8                        | 40.0 |
| 0                             | 1    | 1   | 0   | 2     | 9                        | 45.0 |
| 0                             | 0    | 1   | 0   | 1     | 10                       | 50.0 |
| 0                             | 0    | 1   | 0   | 1     | 11                       | 55.0 |

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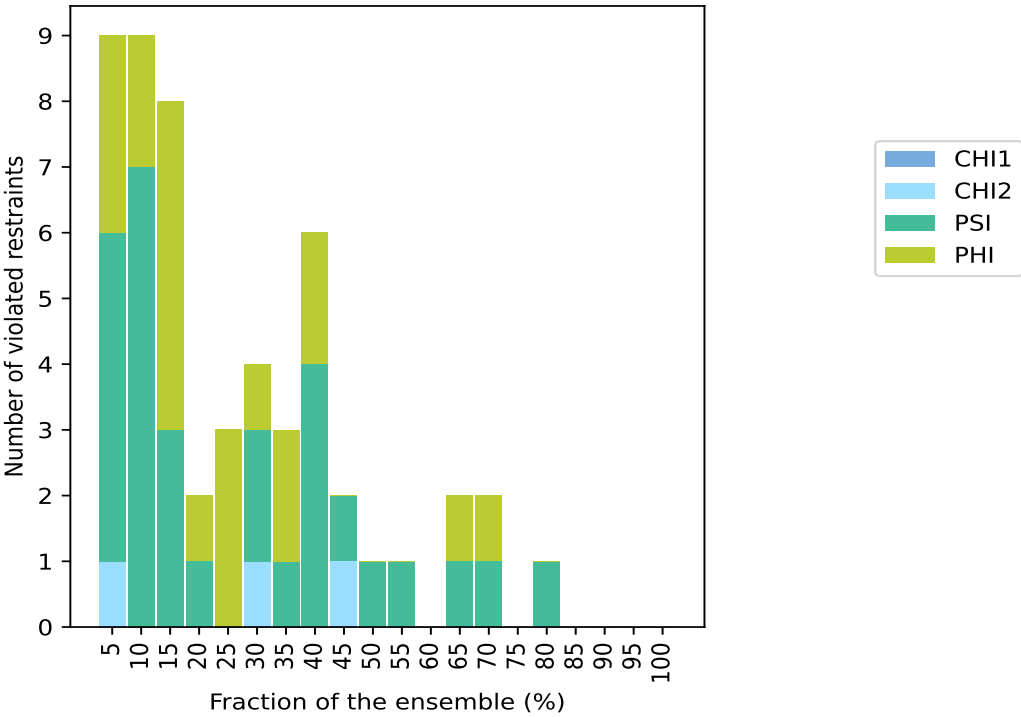


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| Number of violated restraints |      |     |     |       | Fraction of the ensemble |       |
|-------------------------------|------|-----|-----|-------|--------------------------|-------|
| CHI1                          | CHI2 | PSI | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0    | 0   | 0   | 0     | 12                       | 60.0  |
| 0                             | 0    | 1   | 1   | 2     | 13                       | 65.0  |
| 0                             | 0    | 1   | 1   | 2     | 14                       | 70.0  |
| 0                             | 0    | 0   | 0   | 0     | 15                       | 75.0  |
| 0                             | 0    | 1   | 0   | 1     | 16                       | 80.0  |
| 0                             | 0    | 0   | 0   | 0     | 17                       | 85.0  |
| 0                             | 0    | 0   | 0   | 0     | 18                       | 90.0  |
| 0                             | 0    | 0   | 0   | 0     | 19                       | 95.0  |
| 0                             | 0    | 0   | 0   | 0     | 20                       | 100.0 |

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

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

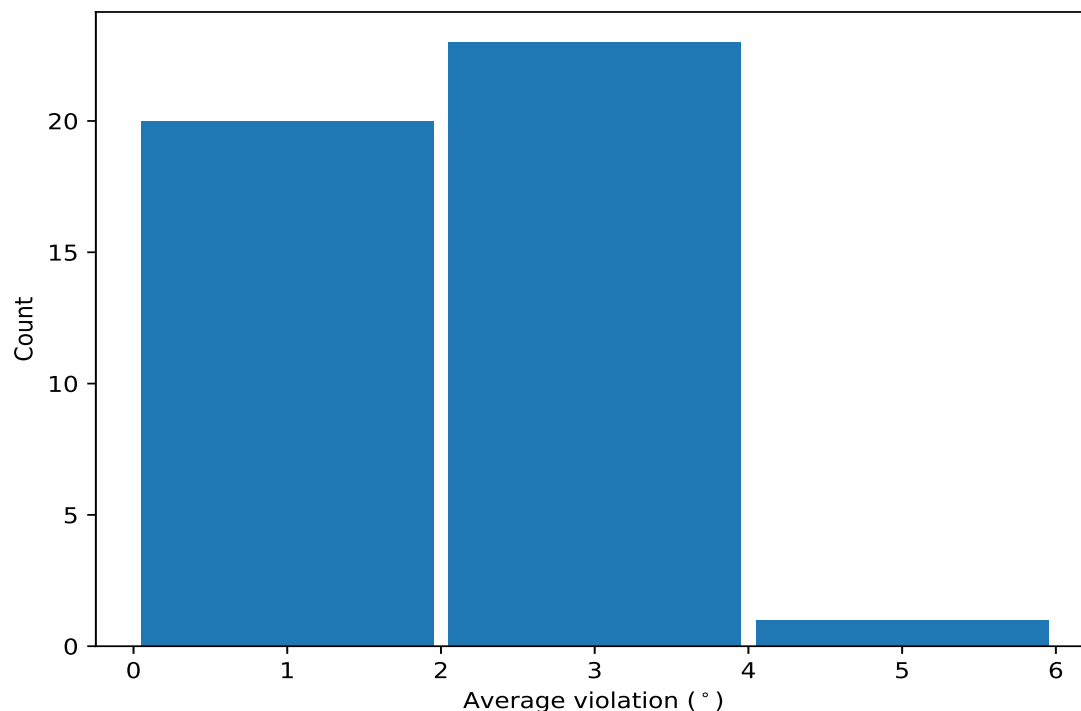


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

| Key    | Atom-1        | Atom-2        | Atom-3        | Atom-4         | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|---------------|---------------|---------------|----------------|---------------------|------|-----------------|--------|
| (1,61) | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 16                  | 3.06 | 1.17            | 3.14   |
| (1,18) | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 14                  | 2.92 | 1.25            | 2.94   |
| (1,27) | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 14                  | 2.87 | 1.17            | 2.61   |
| (1,80) | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 13                  | 3.3  | 1.19            | 3.13   |
| (1,55) | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 13                  | 3.28 | 1.72            | 3.0    |
| (1,77) | 1:53:A:VAL:N  | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N   | 11                  | 3.34 | 1.42            | 3.5    |
| (1,15) | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N   | 10                  | 3.56 | 1.53            | 3.32   |
| (1,13) | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N    | 9                   | 2.51 | 1.25            | 1.96   |
| (1,1)  | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 9                   | 2.25 | 1.07            | 1.41   |
| (1,20) | 1:16:A:GLY:C  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C   | 8                   | 4.7  | 2.41            | 3.71   |
| (1,33) | 1:25:A:ASN:N  | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N   | 8                   | 3.02 | 1.47            | 2.78   |
| (1,21) | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N   | 8                   | 2.67 | 0.54            | 2.52   |
| (1,17) | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N   | 8                   | 2.63 | 1.07            | 2.47   |
| (1,46) | 1:31:A:GLN:C  | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C   | 8                   | 1.85 | 0.6             | 1.86   |
| (1,75) | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N   | 8                   | 1.81 | 0.45            | 1.75   |
| (1,12) | 1:5:A:ALA:C   | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C    | 7                   | 2.09 | 0.67            | 1.91   |
| (1,43) | 1:30:A:ILE:N  | 1:30:A:ILE:CA | 1:30:A:ILE:C  | 1:31:A:GLN:N   | 7                   | 1.73 | 0.52            | 1.42   |
| (1,52) | 1:40:A:PRO:C  | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C   | 7                   | 1.71 | 0.39            | 1.85   |
| (1,5)  | 1:47:A:TRP:CA | 1:47:A:TRP:CB | 1:47:A:TRP:CG | 1:47:A:TRP:CD1 | 6                   | 2.0  | 0.68            | 2.04   |
| (1,19) | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C  | 1:15:A:SER:N   | 6                   | 1.94 | 1.05            | 1.64   |

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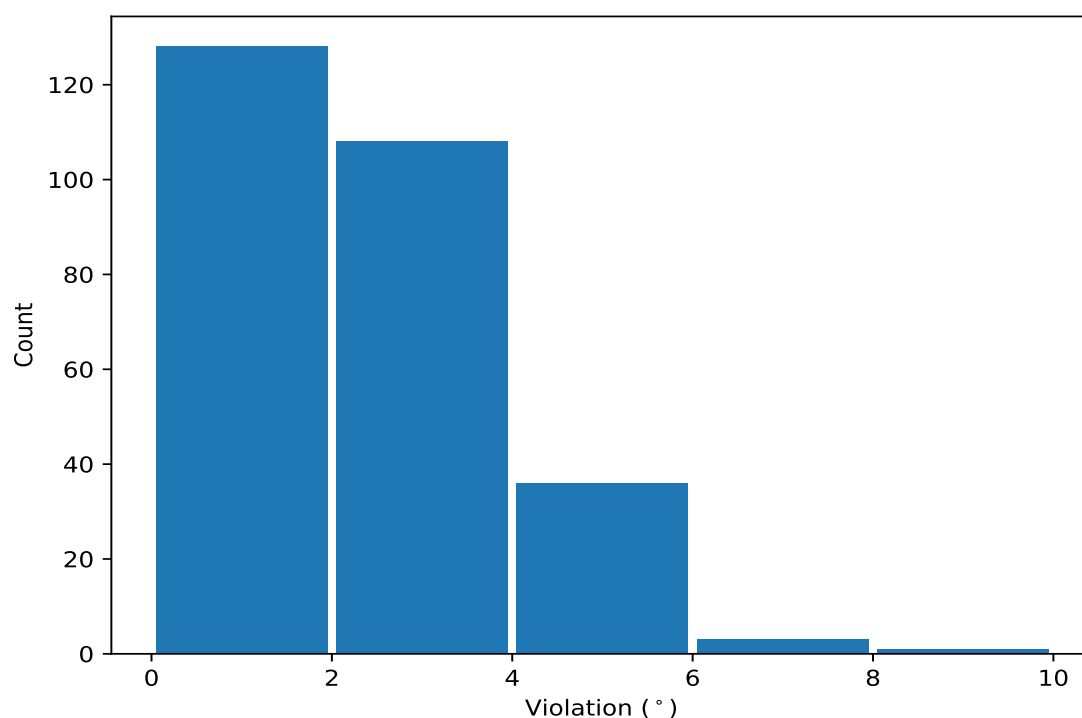
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,53)  | 1:41:A:LYS:N | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:THR:N | 6                   | 1.94 | 0.75            | 1.62   |
| (1,10)  | 1:4:A:GLU:C  | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C  | 6                   | 1.89 | 0.53            | 1.86   |
| (1,50)  | 1:38:A:GLY:C | 1:39:A:CYS:N  | 1:39:A:CYS:CA | 1:39:A:CYS:C | 5                   | 2.43 | 0.91            | 2.62   |
| (1,60)  | 1:44:A:VAL:C | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C | 5                   | 1.91 | 0.79            | 1.97   |
| (1,58)  | 1:43:A:GLU:C | 1:44:A:VAL:N  | 1:44:A:VAL:CA | 1:44:A:VAL:C | 5                   | 1.59 | 0.62            | 1.38   |
| (1,39)  | 1:28:A:ASP:N | 1:28:A:ASP:CA | 1:28:A:ASP:C  | 1:29:A:ARG:N | 4                   | 1.95 | 0.44            | 2.15   |
| (1,8)   | 1:3:A:LEU:C  | 1:4:A:GLU:N   | 1:4:A:GLU:CA  | 1:4:A:GLU:C  | 4                   | 1.92 | 0.43            | 1.85   |
| (1,54)  | 1:41:A:LYS:C | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C | 3                   | 2.61 | 0.56            | 2.32   |
| (1,11)  | 1:5:A:ALA:N  | 1:5:A:ALA:CA  | 1:5:A:ALA:C   | 1:6:A:HIS:N  | 3                   | 2.35 | 1.63            | 1.38   |
| (1,38)  | 1:27:A:ILE:C | 1:28:A:ASP:N  | 1:28:A:ASP:CA | 1:28:A:ASP:C | 3                   | 2.17 | 0.93            | 1.51   |
| (1,16)  | 1:12:A:CYS:C | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C | 3                   | 2.1  | 1.21            | 1.45   |
| (1,59)  | 1:44:A:VAL:N | 1:44:A:VAL:CA | 1:44:A:VAL:C  | 1:45:A:VAL:N | 3                   | 1.99 | 0.06            | 1.99   |
| (1,6)   | 1:2:A:ILE:C  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C  | 3                   | 1.54 | 0.12            | 1.58   |
| (1,83)  | 1:56:A:VAL:N | 1:56:A:VAL:CA | 1:56:A:VAL:C  | 1:57:A:ASN:N | 3                   | 1.51 | 0.36            | 1.5    |
| (1,62)  | 1:45:A:VAL:C | 1:46:A:ILE:N  | 1:46:A:ILE:CA | 1:46:A:ILE:C | 3                   | 1.33 | 0.23            | 1.42   |
| (1,57)  | 1:43:A:GLU:N | 1:43:A:GLU:CA | 1:43:A:GLU:C  | 1:44:A:VAL:N | 2                   | 3.12 | 0.28            | 3.12   |
| (1,105) | 1:67:A:LEU:C | 1:68:A:ARG:N  | 1:68:A:ARG:CA | 1:68:A:ARG:C | 2                   | 3.01 | 0.53            | 3.01   |
| (1,14)  | 1:11:A:LYS:C | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C | 2                   | 2.97 | 1.34            | 2.97   |
| (1,7)   | 1:3:A:LEU:N  | 1:3:A:LEU:CA  | 1:3:A:LEU:C   | 1:4:A:GLU:N  | 2                   | 2.03 | 0.4             | 2.03   |
| (1,9)   | 1:4:A:GLU:N  | 1:4:A:GLU:CA  | 1:4:A:GLU:C   | 1:5:A:ALA:N  | 2                   | 1.75 | 0.26            | 1.75   |
| (1,73)  | 1:51:A:LYS:N | 1:51:A:LYS:CA | 1:51:A:LYS:C  | 1:52:A:LYS:N | 2                   | 1.72 | 0.72            | 1.72   |
| (1,81)  | 1:55:A:CYS:N | 1:55:A:CYS:CA | 1:55:A:CYS:C  | 1:56:A:VAL:N | 2                   | 1.72 | 0.54            | 1.72   |
| (1,51)  | 1:39:A:CYS:N | 1:39:A:CYS:CA | 1:39:A:CYS:C  | 1:40:A:PRO:N | 2                   | 1.42 | 0.26            | 1.42   |
| (1,49)  | 1:33:A:THR:N | 1:33:A:THR:CA | 1:33:A:THR:C  | 1:34:A:PRO:N | 2                   | 1.28 | 0.23            | 1.28   |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,20) | 1:16:A:GLY:C | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C | 13       | 8.31          |
| (1,20) | 1:16:A:GLY:C | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C | 3        | 7.74          |
| (1,20) | 1:16:A:GLY:C | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C | 6        | 7.04          |
| (1,15) | 1:12:A:CYS:N | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N | 16       | 6.55          |
| (1,55) | 1:42:A:THR:N | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N | 20       | 5.94          |
| (1,33) | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N | 17       | 5.87          |
| (1,77) | 1:53:A:VAL:N | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N | 14       | 5.68          |
| (1,55) | 1:42:A:THR:N | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N | 7        | 5.51          |
| (1,15) | 1:12:A:CYS:N | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N | 13       | 5.36          |
| (1,13) | 1:6:A:HIS:N  | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N  | 6        | 5.26          |
| (1,80) | 1:54:A:ILE:C | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C | 12       | 5.21          |
| (1,55) | 1:42:A:THR:N | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N | 11       | 5.21          |
| (1,61) | 1:45:A:VAL:N | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N | 2        | 5.1           |
| (1,55) | 1:42:A:THR:N | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N | 12       | 4.9           |
| (1,27) | 1:21:A:VAL:N | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N | 6        | 4.84          |
| (1,77) | 1:53:A:VAL:N | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N | 15       | 4.79          |
| (1,18) | 1:13:A:ARG:C | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C | 5        | 4.79          |
| (1,61) | 1:45:A:VAL:N | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N | 18       | 4.77          |
| (1,15) | 1:12:A:CYS:N | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N | 11       | 4.75          |
| (1,80) | 1:54:A:ILE:C | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C | 18       | 4.71          |
| (1,18) | 1:13:A:ARG:C | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C | 14       | 4.69          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4         | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|----------------|----------|---------------|
| (1,11)  | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C   | 1:6:A:HIS:N    | 12       | 4.64          |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 11       | 4.63          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 10       | 4.61          |
| (1,77)  | 1:53:A:VAL:N  | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N   | 4        | 4.57          |
| (1,77)  | 1:53:A:VAL:N  | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N   | 3        | 4.55          |
| (1,17)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N   | 14       | 4.55          |
| (1,80)  | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 20       | 4.53          |
| (1,18)  | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 3        | 4.52          |
| (1,80)  | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 11       | 4.44          |
| (1,33)  | 1:25:A:ASN:N  | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N   | 14       | 4.36          |
| (1,55)  | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 16       | 4.33          |
| (1,14)  | 1:11:A:LYS:C  | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C   | 14       | 4.31          |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 1        | 4.24          |
| (1,19)  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C  | 1:15:A:SER:N   | 4        | 4.22          |
| (1,55)  | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 8        | 4.21          |
| (1,1)   | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 9        | 4.14          |
| (1,18)  | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 20       | 4.11          |
| (1,15)  | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N   | 10       | 4.04          |
| (1,80)  | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 14       | 4.02          |
| (1,77)  | 1:53:A:VAL:N  | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N   | 9        | 3.98          |
| (1,20)  | 1:16:A:GLY:C  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C   | 17       | 3.97          |
| (1,18)  | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 16       | 3.94          |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 18       | 3.89          |
| (1,50)  | 1:38:A:GLY:C  | 1:39:A:CYS:N  | 1:39:A:CYS:CA | 1:39:A:CYS:C   | 18       | 3.81          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 3        | 3.8           |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 13       | 3.8           |
| (1,16)  | 1:12:A:CYS:C  | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C   | 10       | 3.8           |
| (1,13)  | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N    | 3        | 3.71          |
| (1,80)  | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 10       | 3.65          |
| (1,33)  | 1:25:A:ASN:N  | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N   | 8        | 3.63          |
| (1,17)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N   | 20       | 3.6           |
| (1,1)   | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 3        | 3.59          |
| (1,15)  | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N   | 4        | 3.58          |
| (1,21)  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N   | 13       | 3.55          |
| (1,105) | 1:67:A:LEU:C  | 1:68:A:ARG:N  | 1:68:A:ARG:CA | 1:68:A:ARG:C   | 11       | 3.54          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 4        | 3.54          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 12       | 3.52          |
| (1,77)  | 1:53:A:VAL:N  | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N   | 2        | 3.5           |
| (1,38)  | 1:27:A:ILE:C  | 1:28:A:ASP:N  | 1:28:A:ASP:CA | 1:28:A:ASP:C   | 4        | 3.49          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 14       | 3.46          |
| (1,20)  | 1:16:A:GLY:C  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C   | 10       | 3.45          |
| (1,21)  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N   | 5        | 3.41          |
| (1,57)  | 1:43:A:GLU:N  | 1:43:A:GLU:CA | 1:43:A:GLU:C  | 1:44:A:VAL:N   | 2        | 3.4           |
| (1,54)  | 1:41:A:LYS:C  | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C   | 16       | 3.4           |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 1        | 3.37          |
| (1,17)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N   | 16       | 3.35          |
| (1,60)  | 1:44:A:VAL:C  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C   | 10       | 3.27          |
| (1,13)  | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N    | 4        | 3.17          |
| (1,1)   | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 2        | 3.17          |
| (1,80)  | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 4        | 3.13          |
| (1,80)  | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 8        | 3.09          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4         | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|----------------|----------|---------------|
| (1,15)  | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N   | 20       | 3.05          |
| (1,12)  | 1:5:A:ALA:C   | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C    | 7        | 3.04          |
| (1,80)  | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 6        | 3.02          |
| (1,55)  | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 6        | 3.0           |
| (1,12)  | 1:5:A:ALA:C   | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C    | 12       | 3.0           |
| (1,53)  | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:THR:N   | 1        | 2.98          |
| (1,18)  | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 9        | 2.97          |
| (1,53)  | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:THR:N   | 7        | 2.95          |
| (1,33)  | 1:25:A:ASN:N  | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N   | 10       | 2.95          |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 5        | 2.95          |
| (1,18)  | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 19       | 2.95          |
| (1,5)   | 1:47:A:TRP:CA | 1:47:A:TRP:CB | 1:47:A:TRP:CG | 1:47:A:TRP:CD1 | 12       | 2.95          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 6        | 2.92          |
| (1,18)  | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 11       | 2.92          |
| (1,21)  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N   | 6        | 2.91          |
| (1,57)  | 1:43:A:GLU:N  | 1:43:A:GLU:CA | 1:43:A:GLU:C  | 1:44:A:VAL:N   | 11       | 2.83          |
| (1,46)  | 1:31:A:GLN:C  | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C   | 16       | 2.83          |
| (1,10)  | 1:4:A:GLU:C   | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C    | 1        | 2.83          |
| (1,58)  | 1:43:A:GLU:C  | 1:44:A:VAL:N  | 1:44:A:VAL:CA | 1:44:A:VAL:C   | 16       | 2.82          |
| (1,50)  | 1:38:A:GLY:C  | 1:39:A:CYS:N  | 1:39:A:CYS:CA | 1:39:A:CYS:C   | 11       | 2.79          |
| (1,17)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N   | 9        | 2.79          |
| (1,77)  | 1:53:A:VAL:N  | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N   | 11       | 2.78          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 8        | 2.7           |
| (1,43)  | 1:30:A:ILE:N  | 1:30:A:ILE:CA | 1:30:A:ILE:C  | 1:31:A:GLN:N   | 17       | 2.69          |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 2        | 2.69          |
| (1,21)  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N   | 19       | 2.64          |
| (1,50)  | 1:38:A:GLY:C  | 1:39:A:CYS:N  | 1:39:A:CYS:CA | 1:39:A:CYS:C   | 5        | 2.62          |
| (1,33)  | 1:25:A:ASN:N  | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N   | 2        | 2.62          |
| (1,20)  | 1:16:A:GLY:C  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C   | 11       | 2.56          |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 17       | 2.53          |
| (1,20)  | 1:16:A:GLY:C  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C   | 20       | 2.53          |
| (1,5)   | 1:47:A:TRP:CA | 1:47:A:TRP:CB | 1:47:A:TRP:CG | 1:47:A:TRP:CD1 | 3        | 2.52          |
| (1,15)  | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N   | 9        | 2.51          |
| (1,8)   | 1:3:A:LEU:C   | 1:4:A:GLU:N   | 1:4:A:GLU:CA  | 1:4:A:GLU:C    | 14       | 2.5           |
| (1,1)   | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 11       | 2.5           |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 17       | 2.49          |
| (1,105) | 1:67:A:LEU:C  | 1:68:A:ARG:N  | 1:68:A:ARG:CA | 1:68:A:ARG:C   | 10       | 2.48          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 7        | 2.48          |
| (1,75)  | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N   | 4        | 2.46          |
| (1,73)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA | 1:51:A:LYS:C  | 1:52:A:LYS:N   | 15       | 2.44          |
| (1,5)   | 1:47:A:TRP:CA | 1:47:A:TRP:CB | 1:47:A:TRP:CG | 1:47:A:TRP:CD1 | 1        | 2.44          |
| (1,15)  | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N   | 3        | 2.43          |
| (1,7)   | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C   | 1:4:A:GLU:N    | 3        | 2.43          |
| (1,21)  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N   | 16       | 2.4           |
| (1,46)  | 1:31:A:GLN:C  | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C   | 11       | 2.39          |
| (1,21)  | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N   | 8        | 2.39          |
| (1,55)  | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 18       | 2.36          |
| (1,12)  | 1:5:A:ALA:C   | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C    | 8        | 2.34          |
| (1,75)  | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N   | 7        | 2.33          |
| (1,13)  | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N    | 7        | 2.33          |
| (1,54)  | 1:41:A:LYS:C  | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C   | 11       | 2.32          |

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| Key    | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,39) | 1:28:A:ASP:N | 1:28:A:ASP:CA | 1:28:A:ASP:C  | 1:29:A:ARG:N | 14       | 2.3           |
| (1,61) | 1:45:A:VAL:N | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N | 9        | 2.28          |
| (1,46) | 1:31:A:GLN:C | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C | 17       | 2.27          |
| (1,81) | 1:55:A:CYS:N | 1:55:A:CYS:CA | 1:55:A:CYS:C  | 1:56:A:VAL:N | 18       | 2.26          |
| (1,18) | 1:13:A:ARG:C | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C | 10       | 2.25          |
| (1,75) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 14       | 2.22          |
| (1,27) | 1:21:A:VAL:N | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N | 7        | 2.21          |
| (1,39) | 1:28:A:ASP:N | 1:28:A:ASP:CA | 1:28:A:ASP:C  | 1:29:A:ARG:N | 12       | 2.2           |
| (1,10) | 1:4:A:GLU:C  | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C  | 4        | 2.18          |
| (1,43) | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C  | 1:31:A:GLN:N | 1        | 2.17          |
| (1,8)  | 1:3:A:LEU:C  | 1:4:A:GLU:N   | 1:4:A:GLU:CA  | 1:4:A:GLU:C  | 8        | 2.16          |
| (1,17) | 1:13:A:ARG:N | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N | 10       | 2.15          |
| (1,46) | 1:31:A:GLN:C | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C | 14       | 2.14          |
| (1,54) | 1:41:A:LYS:C | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C | 8        | 2.12          |
| (1,52) | 1:40:A:PRO:C | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C | 13       | 2.12          |
| (1,52) | 1:40:A:PRO:C | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C | 15       | 2.1           |
| (1,39) | 1:28:A:ASP:N | 1:28:A:ASP:CA | 1:28:A:ASP:C  | 1:29:A:ARG:N | 2        | 2.1           |
| (1,33) | 1:25:A:ASN:N | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N | 16       | 2.09          |
| (1,21) | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N | 2        | 2.08          |
| (1,59) | 1:44:A:VAL:N | 1:44:A:VAL:CA | 1:44:A:VAL:C  | 1:45:A:VAL:N | 2        | 2.07          |
| (1,60) | 1:44:A:VAL:C | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C | 14       | 2.05          |
| (1,27) | 1:21:A:VAL:N | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N | 10       | 2.03          |
| (1,43) | 1:30:A:ILE:N | 1:30:A:ILE:CA | 1:30:A:ILE:C  | 1:31:A:GLN:N | 19       | 2.02          |
| (1,20) | 1:16:A:GLY:C | 1:17:A:VAL:N  | 1:17:A:VAL:CA | 1:17:A:VAL:C | 8        | 2.01          |
| (1,9)  | 1:4:A:GLU:N  | 1:4:A:GLU:CA  | 1:4:A:GLU:C   | 1:5:A:ALA:N  | 14       | 2.01          |
| (1,59) | 1:44:A:VAL:N | 1:44:A:VAL:CA | 1:44:A:VAL:C  | 1:45:A:VAL:N | 6        | 1.99          |
| (1,79) | 1:54:A:ILE:N | 1:54:A:ILE:CA | 1:54:A:ILE:C  | 1:55:A:CYS:N | 4        | 1.98          |
| (1,21) | 1:17:A:VAL:N | 1:17:A:VAL:CA | 1:17:A:VAL:C  | 1:18:A:ILE:N | 14       | 1.98          |
| (1,60) | 1:44:A:VAL:C | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C | 7        | 1.97          |
| (1,27) | 1:21:A:VAL:N | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N | 12       | 1.97          |
| (1,83) | 1:56:A:VAL:N | 1:56:A:VAL:CA | 1:56:A:VAL:C  | 1:57:A:ASN:N | 16       | 1.96          |
| (1,18) | 1:13:A:ARG:C | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C | 7        | 1.96          |
| (1,13) | 1:6:A:HIS:N  | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N  | 13       | 1.96          |
| (1,80) | 1:54:A:ILE:C | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C | 13       | 1.95          |
| (1,59) | 1:44:A:VAL:N | 1:44:A:VAL:CA | 1:44:A:VAL:C  | 1:45:A:VAL:N | 7        | 1.92          |
| (1,52) | 1:40:A:PRO:C | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C | 19       | 1.91          |
| (1,12) | 1:5:A:ALA:C  | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C  | 15       | 1.91          |
| (1,77) | 1:53:A:VAL:N | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N | 1        | 1.9           |
| (1,10) | 1:4:A:GLU:C  | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C  | 15       | 1.9           |
| (1,27) | 1:21:A:VAL:N | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N | 3        | 1.89          |
| (1,77) | 1:53:A:VAL:N | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N | 5        | 1.87          |
| (1,52) | 1:40:A:PRO:C | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C | 18       | 1.85          |
| (1,77) | 1:53:A:VAL:N | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N | 7        | 1.84          |
| (1,40) | 1:28:A:ASP:C | 1:29:A:ARG:N  | 1:29:A:ARG:CA | 1:29:A:ARG:C | 11       | 1.84          |
| (1,13) | 1:6:A:HIS:N  | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N  | 1        | 1.84          |
| (1,13) | 1:6:A:HIS:N  | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N  | 15       | 1.84          |
| (1,75) | 1:52:A:LYS:N | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N | 19       | 1.82          |
| (1,10) | 1:4:A:GLU:C  | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C  | 2        | 1.82          |
| (1,50) | 1:38:A:GLY:C | 1:39:A:CYS:N  | 1:39:A:CYS:CA | 1:39:A:CYS:C | 10       | 1.79          |
| (1,80) | 1:54:A:ILE:C | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C | 5        | 1.76          |
| (1,18) | 1:13:A:ARG:C | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C | 8        | 1.76          |

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| Key    | Atom-1        | Atom-2        | Atom-3        | Atom-4         | Model ID | Violation (°) |
|--------|---------------|---------------|---------------|----------------|----------|---------------|
| (1,12) | 1:5:A:ALA:C   | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C    | 20       | 1.75          |
| (1,15) | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N   | 6        | 1.74          |
| (1,53) | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:THR:N   | 6        | 1.73          |
| (1,17) | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N   | 3        | 1.73          |
| (1,19) | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C  | 1:15:A:SER:N   | 17       | 1.72          |
| (1,52) | 1:40:A:PRO:C  | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C   | 1        | 1.71          |
| (1,17) | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N   | 5        | 1.71          |
| (1,80) | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 2        | 1.7           |
| (1,80) | 1:54:A:ILE:C  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C   | 9        | 1.7           |
| (1,55) | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 14       | 1.69          |
| (1,75) | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N   | 5        | 1.68          |
| (1,51) | 1:39:A:CYS:N  | 1:39:A:CYS:CA | 1:39:A:CYS:C  | 1:40:A:PRO:N   | 12       | 1.68          |
| (1,19) | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C  | 1:15:A:SER:N   | 5        | 1.66          |
| (1,6)  | 1:2:A:ILE:C   | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C    | 19       | 1.66          |
| (1,5)  | 1:47:A:TRP:CA | 1:47:A:TRP:CB | 1:47:A:TRP:CG | 1:47:A:TRP:CD1 | 6        | 1.65          |
| (1,15) | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C  | 1:13:A:ARG:N   | 8        | 1.64          |
| (1,14) | 1:11:A:LYS:C  | 1:12:A:CYS:N  | 1:12:A:CYS:CA | 1:12:A:CYS:C   | 19       | 1.63          |
| (1,19) | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C  | 1:15:A:SER:N   | 15       | 1.62          |
| (1,7)  | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C   | 1:4:A:GLU:N    | 11       | 1.62          |
| (1,46) | 1:31:A:GLN:C  | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C   | 1        | 1.58          |
| (1,6)  | 1:2:A:ILE:C   | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C    | 17       | 1.58          |
| (1,62) | 1:45:A:VAL:C  | 1:46:A:ILE:N  | 1:46:A:ILE:CA | 1:46:A:ILE:C   | 13       | 1.55          |
| (1,8)  | 1:3:A:LEU:C   | 1:4:A:GLU:N   | 1:4:A:GLU:CA  | 1:4:A:GLU:C    | 16       | 1.53          |
| (1,49) | 1:33:A:THR:N  | 1:33:A:THR:CA | 1:33:A:THR:C  | 1:34:A:PRO:N   | 8        | 1.51          |
| (1,38) | 1:27:A:ILE:C  | 1:28:A:ASP:N  | 1:28:A:ASP:CA | 1:28:A:ASP:C   | 1        | 1.51          |
| (1,38) | 1:27:A:ILE:C  | 1:28:A:ASP:N  | 1:28:A:ASP:CA | 1:28:A:ASP:C   | 19       | 1.51          |
| (1,83) | 1:56:A:VAL:N  | 1:56:A:VAL:CA | 1:56:A:VAL:C  | 1:57:A:ASN:N   | 5        | 1.5           |
| (1,53) | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:THR:N   | 20       | 1.5           |
| (1,18) | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 12       | 1.5           |
| (1,55) | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 4        | 1.49          |
| (1,13) | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N    | 2        | 1.49          |
| (1,9)  | 1:4:A:GLU:N   | 1:4:A:GLU:CA  | 1:4:A:GLU:C   | 1:5:A:ALA:N    | 20       | 1.49          |
| (1,55) | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 1        | 1.48          |
| (1,45) | 1:31:A:GLN:N  | 1:31:A:GLN:CA | 1:31:A:GLN:C  | 1:32:A:VAL:N   | 3        | 1.48          |
| (1,8)  | 1:3:A:LEU:C   | 1:4:A:GLU:N   | 1:4:A:GLU:CA  | 1:4:A:GLU:C    | 20       | 1.47          |
| (1,16) | 1:12:A:CYS:C  | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C   | 5        | 1.45          |
| (1,33) | 1:25:A:ASN:N  | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N   | 9        | 1.44          |
| (1,75) | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N   | 2        | 1.43          |
| (1,62) | 1:45:A:VAL:C  | 1:46:A:ILE:N  | 1:46:A:ILE:CA | 1:46:A:ILE:C   | 7        | 1.42          |
| (1,61) | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 5        | 1.42          |
| (1,61) | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 16       | 1.42          |
| (1,43) | 1:30:A:ILE:N  | 1:30:A:ILE:CA | 1:30:A:ILE:C  | 1:31:A:GLN:N   | 12       | 1.42          |
| (1,18) | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 1        | 1.42          |
| (1,1)  | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 20       | 1.41          |
| (1,58) | 1:43:A:GLU:C  | 1:44:A:VAL:N  | 1:44:A:VAL:CA | 1:44:A:VAL:C   | 5        | 1.4           |
| (1,75) | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N   | 17       | 1.39          |
| (1,12) | 1:5:A:ALA:C   | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C    | 16       | 1.39          |
| (1,10) | 1:4:A:GLU:C   | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C    | 9        | 1.39          |
| (1,58) | 1:43:A:GLU:C  | 1:44:A:VAL:N  | 1:44:A:VAL:CA | 1:44:A:VAL:C   | 8        | 1.38          |
| (1,11) | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C   | 1:6:A:HIS:N    | 15       | 1.38          |
| (1,1)  | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 13       | 1.38          |

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| Key     | Atom-1        | Atom-2        | Atom-3        | Atom-4         | Model ID | Violation (°) |
|---------|---------------|---------------|---------------|----------------|----------|---------------|
| (1,55)  | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 2        | 1.37          |
| (1,6)   | 1:2:A:ILE:C   | 1:3:A:LEU:N   | 1:3:A:LEU:CA  | 1:3:A:LEU:C    | 6        | 1.37          |
| (1,5)   | 1:47:A:TRP:CA | 1:47:A:TRP:CB | 1:47:A:TRP:CG | 1:47:A:TRP:CD1 | 17       | 1.37          |
| (1,1)   | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 1        | 1.36          |
| (1,1)   | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 7        | 1.36          |
| (1,19)  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C  | 1:15:A:SER:N   | 16       | 1.35          |
| (1,69)  | 1:49:A:LYS:N  | 1:49:A:LYS:CA | 1:49:A:LYS:C  | 1:50:A:MET:N   | 8        | 1.33          |
| (1,43)  | 1:30:A:ILE:N  | 1:30:A:ILE:CA | 1:30:A:ILE:C  | 1:31:A:GLN:N   | 20       | 1.32          |
| (1,43)  | 1:30:A:ILE:N  | 1:30:A:ILE:CA | 1:30:A:ILE:C  | 1:31:A:GLN:N   | 6        | 1.31          |
| (1,1)   | 1:10:A:LEU:CA | 1:10:A:LEU:CB | 1:10:A:LEU:CG | 1:10:A:LEU:CD1 | 17       | 1.3           |
| (1,48)  | 1:32:A:VAL:C  | 1:33:A:THR:N  | 1:33:A:THR:CA | 1:33:A:THR:C   | 9        | 1.29          |
| (1,77)  | 1:53:A:VAL:N  | 1:53:A:VAL:CA | 1:53:A:VAL:C  | 1:54:A:ILE:N   | 17       | 1.27          |
| (1,46)  | 1:31:A:GLN:C  | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C   | 5        | 1.27          |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 19       | 1.27          |
| (1,46)  | 1:31:A:GLN:C  | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C   | 20       | 1.25          |
| (1,53)  | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:THR:N   | 2        | 1.23          |
| (1,27)  | 1:21:A:VAL:N  | 1:21:A:VAL:CA | 1:21:A:VAL:C  | 1:22:A:VAL:N   | 14       | 1.23          |
| (1,12)  | 1:5:A:ALA:C   | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C    | 6        | 1.23          |
| (1,60)  | 1:44:A:VAL:C  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C   | 8        | 1.22          |
| (1,53)  | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:THR:N   | 13       | 1.22          |
| (1,10)  | 1:4:A:GLU:C   | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C    | 17       | 1.21          |
| (1,55)  | 1:42:A:THR:N  | 1:42:A:THR:CA | 1:42:A:THR:C  | 1:43:A:GLU:N   | 9        | 1.2           |
| (1,52)  | 1:40:A:PRO:C  | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C   | 16       | 1.2           |
| (1,43)  | 1:30:A:ILE:N  | 1:30:A:ILE:CA | 1:30:A:ILE:C  | 1:31:A:GLN:N   | 8        | 1.2           |
| (1,39)  | 1:28:A:ASP:N  | 1:28:A:ASP:CA | 1:28:A:ASP:C  | 1:29:A:ARG:N   | 1        | 1.19          |
| (1,81)  | 1:55:A:CYS:N  | 1:55:A:CYS:CA | 1:55:A:CYS:C  | 1:56:A:VAL:N   | 12       | 1.18          |
| (1,17)  | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C  | 1:14:A:CYS:N   | 17       | 1.18          |
| (1,58)  | 1:43:A:GLU:C  | 1:44:A:VAL:N  | 1:44:A:VAL:CA | 1:44:A:VAL:C   | 11       | 1.17          |
| (1,58)  | 1:43:A:GLU:C  | 1:44:A:VAL:N  | 1:44:A:VAL:CA | 1:44:A:VAL:C   | 14       | 1.17          |
| (1,33)  | 1:25:A:ASN:N  | 1:25:A:ASN:CA | 1:25:A:ASN:C  | 1:26:A:ILE:N   | 5        | 1.17          |
| (1,75)  | 1:52:A:LYS:N  | 1:52:A:LYS:CA | 1:52:A:LYS:C  | 1:53:A:VAL:N   | 8        | 1.15          |
| (1,56)  | 1:42:A:THR:C  | 1:43:A:GLU:N  | 1:43:A:GLU:CA | 1:43:A:GLU:C   | 5        | 1.15          |
| (1,51)  | 1:39:A:CYS:N  | 1:39:A:CYS:CA | 1:39:A:CYS:C  | 1:40:A:PRO:N   | 16       | 1.15          |
| (1,18)  | 1:13:A:ARG:C  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C   | 15       | 1.14          |
| (1,50)  | 1:38:A:GLY:C  | 1:39:A:CYS:N  | 1:39:A:CYS:CA | 1:39:A:CYS:C   | 19       | 1.13          |
| (1,110) | 1:70:A:VAL:N  | 1:70:A:VAL:CA | 1:70:A:VAL:C  | 1:71:A:GLN:N   | 8        | 1.12          |
| (1,83)  | 1:56:A:VAL:N  | 1:56:A:VAL:CA | 1:56:A:VAL:C  | 1:57:A:ASN:N   | 10       | 1.07          |
| (1,16)  | 1:12:A:CYS:C  | 1:13:A:ARG:N  | 1:13:A:ARG:CA | 1:13:A:ARG:C   | 17       | 1.06          |
| (1,52)  | 1:40:A:PRO:C  | 1:41:A:LYS:N  | 1:41:A:LYS:CA | 1:41:A:LYS:C   | 4        | 1.05          |
| (1,49)  | 1:33:A:THR:N  | 1:33:A:THR:CA | 1:33:A:THR:C  | 1:34:A:PRO:N   | 2        | 1.05          |
| (1,46)  | 1:31:A:GLN:C  | 1:32:A:VAL:N  | 1:32:A:VAL:CA | 1:32:A:VAL:C   | 10       | 1.05          |
| (1,19)  | 1:14:A:CYS:N  | 1:14:A:CYS:CA | 1:14:A:CYS:C  | 1:15:A:SER:N   | 10       | 1.05          |
| (1,5)   | 1:47:A:TRP:CA | 1:47:A:TRP:CB | 1:47:A:TRP:CG | 1:47:A:TRP:CD1 | 11       | 1.04          |
| (1,2)   | 1:63:A:LEU:CA | 1:63:A:LEU:CB | 1:63:A:LEU:CG | 1:63:A:LEU:CD1 | 2        | 1.04          |
| (1,60)  | 1:44:A:VAL:C  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C   | 15       | 1.03          |
| (1,108) | 1:69:A:HIS:N  | 1:69:A:HIS:CA | 1:69:A:HIS:C  | 1:70:A:VAL:N   | 9        | 1.02          |
| (1,11)  | 1:5:A:ALA:N   | 1:5:A:ALA:CA  | 1:5:A:ALA:C   | 1:6:A:HIS:N    | 3        | 1.02          |
| (1,62)  | 1:45:A:VAL:C  | 1:46:A:ILE:N  | 1:46:A:ILE:CA | 1:46:A:ILE:C   | 17       | 1.01          |
| (1,61)  | 1:45:A:VAL:N  | 1:45:A:VAL:CA | 1:45:A:VAL:C  | 1:46:A:ILE:N   | 13       | 1.01          |
| (1,13)  | 1:6:A:HIS:N   | 1:6:A:HIS:CA  | 1:6:A:HIS:C   | 1:7:A:TYR:N    | 18       | 1.01          |
| (1,73)  | 1:51:A:LYS:N  | 1:51:A:LYS:CA | 1:51:A:LYS:C  | 1:52:A:LYS:N   | 5        | 1.0           |