



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:12 AM UTC

PDB ID : 5GJJ / pdb\_00005gjj  
BMRB ID : 36010  
Title : Glutathionylated hHsp70 SBD  
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Deposited on : 2016-06-30

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  
Mogul : 2022.3.0, CSD as543be (2022)  
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

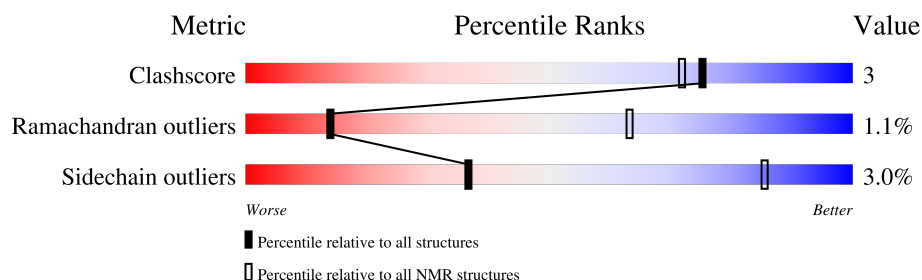
# 1 Overall quality at a glance

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     | 257    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:10-A:121, A:130-A:160<br>(143) | 1.17              | 13           |

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 1 clusters and 1 single-model cluster was found.

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

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

There is only 1 type of molecule in this entry. The entry contains 3902 atoms, of which 1951 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock 70 kDa protein 1A.

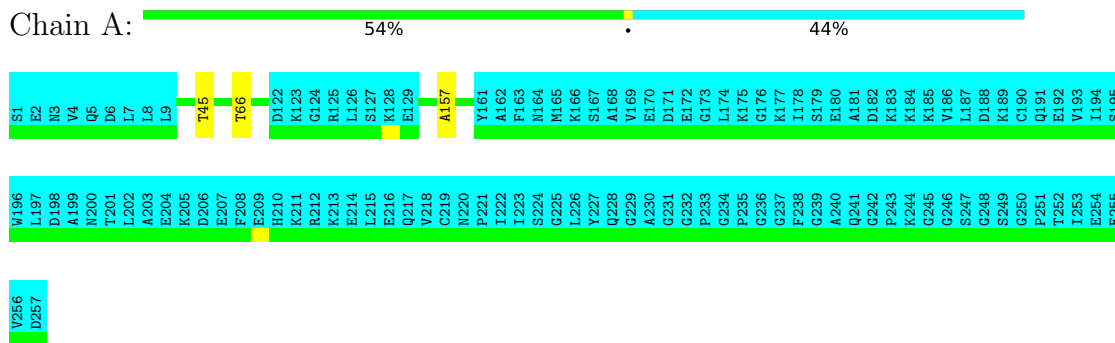
| Mol | Chain | Residues | Atoms |      |      |     |     |   | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
| 1   | A     | 257      | Total | C    | H    | N   | O   | S | 0     |
|     |       |          | 3902  | 1210 | 1951 | 334 | 401 | 6 |       |

## 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: Heat shock 70 kDa protein 1A

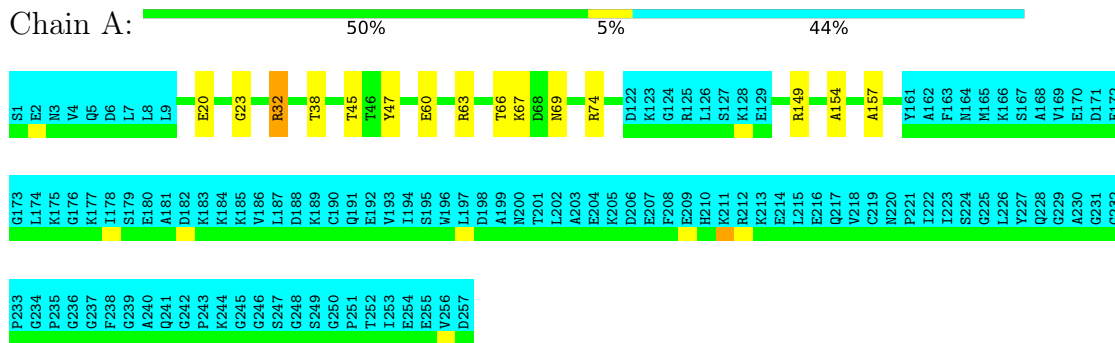


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

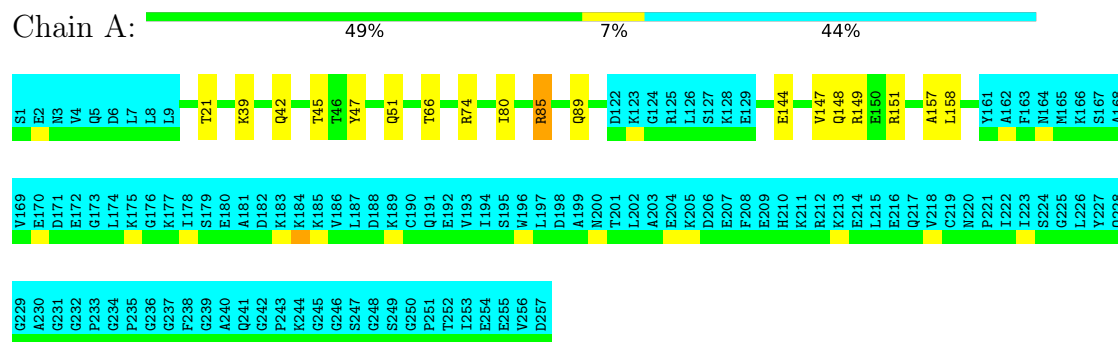
#### 4.2.1 Score per residue for model 1

- Molecule 1: Heat shock 70 kDa protein 1A



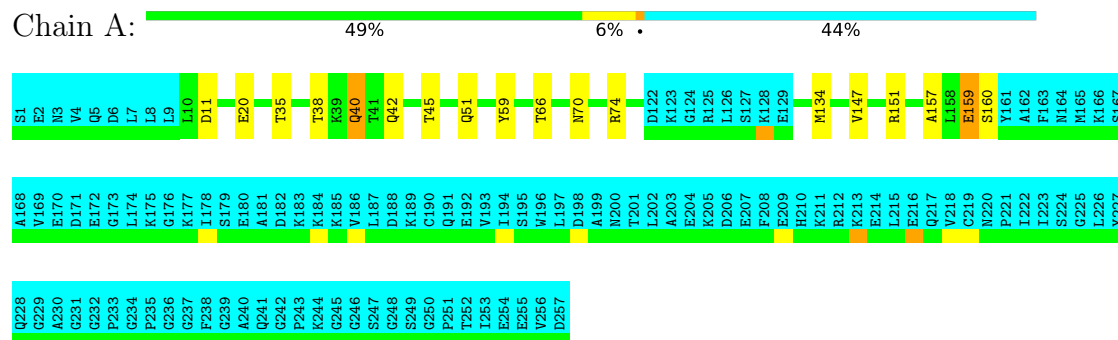
### 4.2.2 Score per residue for model 2

- Molecule 1: Heat shock 70 kDa protein 1A



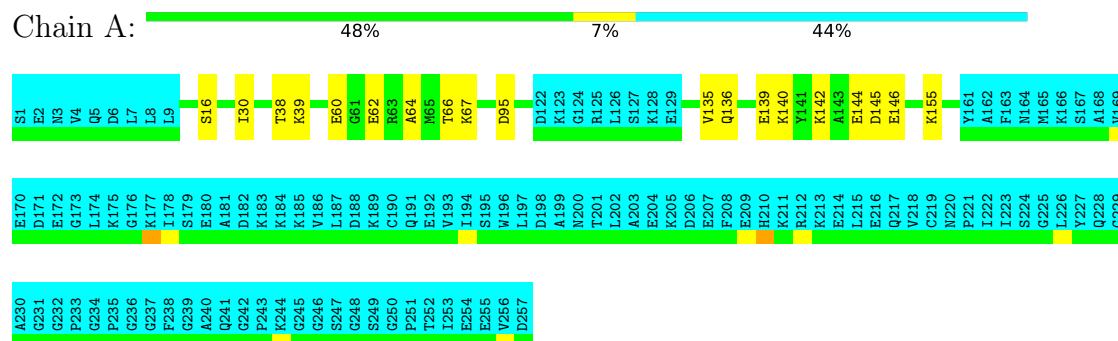
### 4.2.3 Score per residue for model 3

- Molecule 1: Heat shock 70 kDa protein 1A



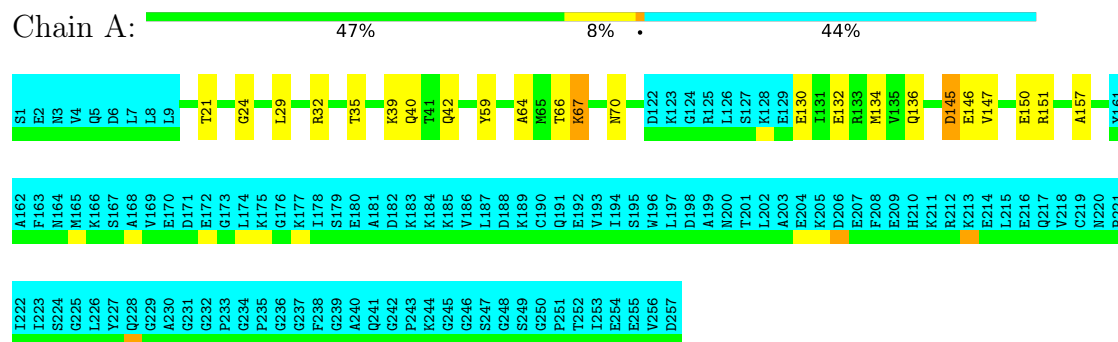
### 4.2.4 Score per residue for model 4

- Molecule 1: Heat shock 70 kDa protein 1A



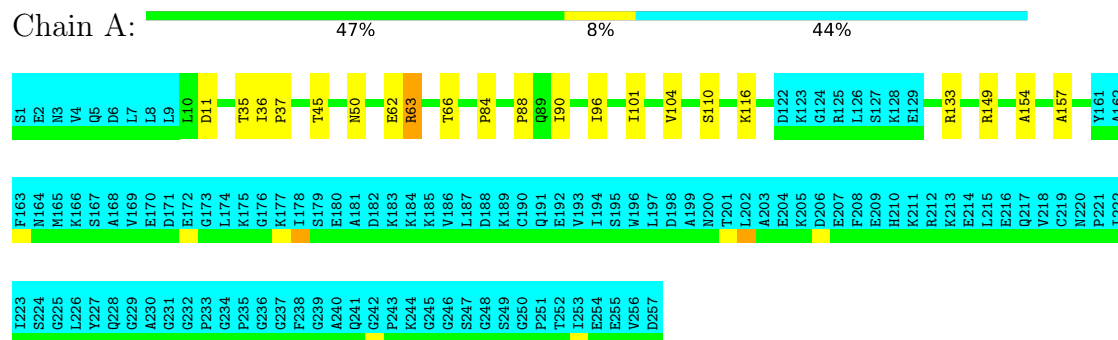
### 4.2.5 Score per residue for model 5

- Molecule 1: Heat shock 70 kDa protein 1A



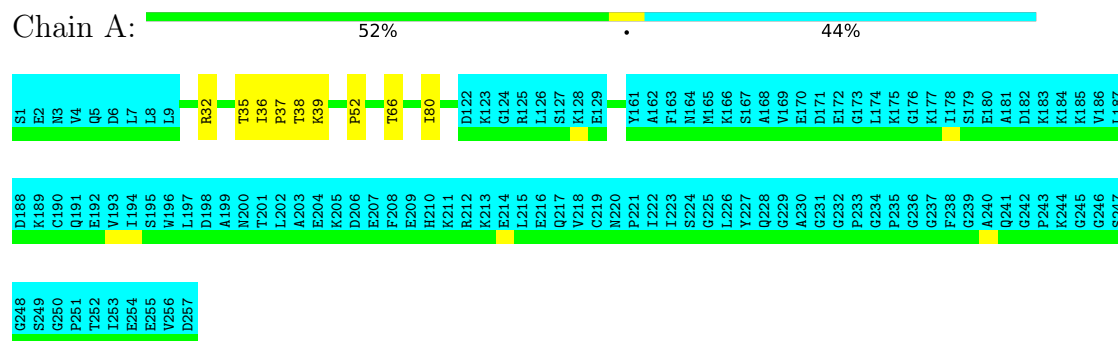
### 4.2.6 Score per residue for model 6

- Molecule 1: Heat shock 70 kDa protein 1A



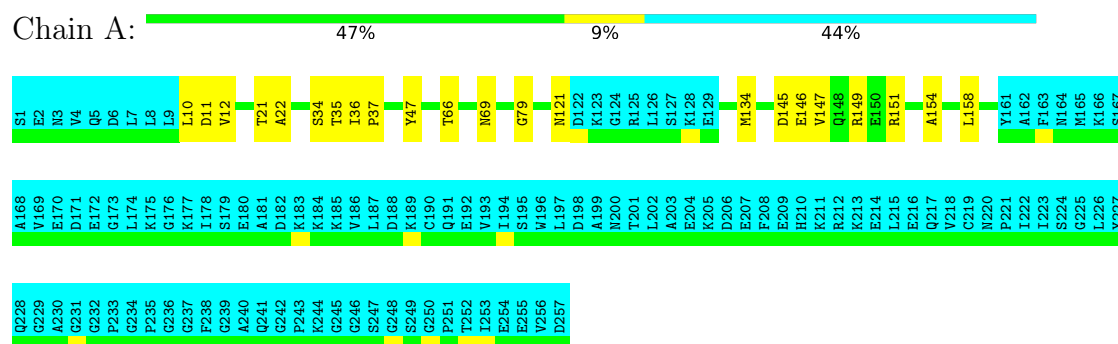
### 4.2.7 Score per residue for model 7

- Molecule 1: Heat shock 70 kDa protein 1A



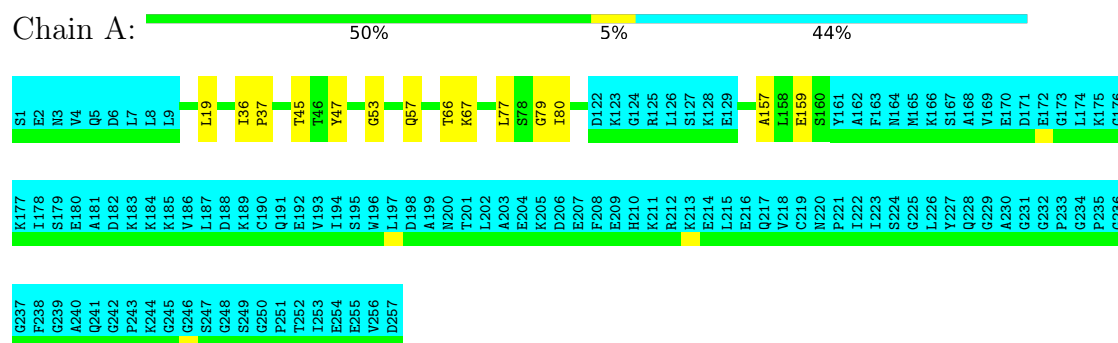
### 4.2.8 Score per residue for model 8

- Molecule 1: Heat shock 70 kDa protein 1A



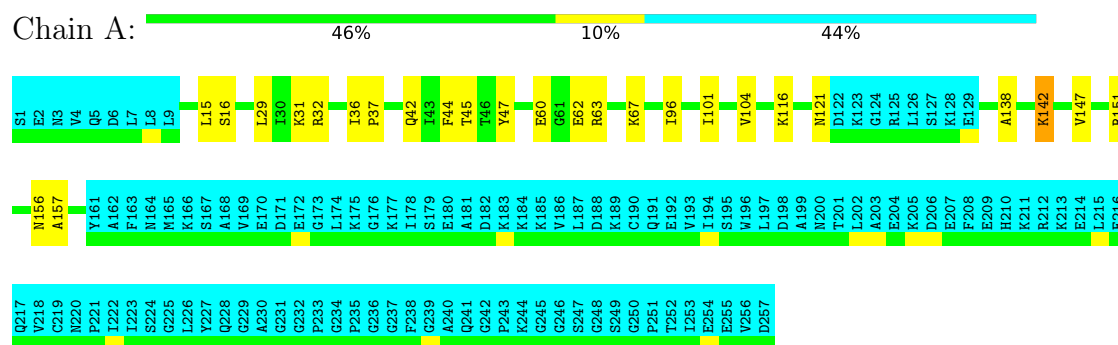
### 4.2.9 Score per residue for model 9

- Molecule 1: Heat shock 70 kDa protein 1A



### 4.2.10 Score per residue for model 10

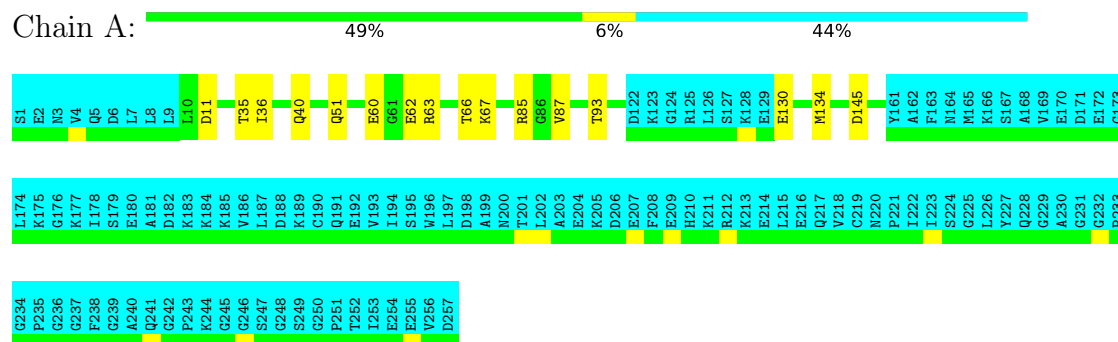
- Molecule 1: Heat shock 70 kDa protein 1A





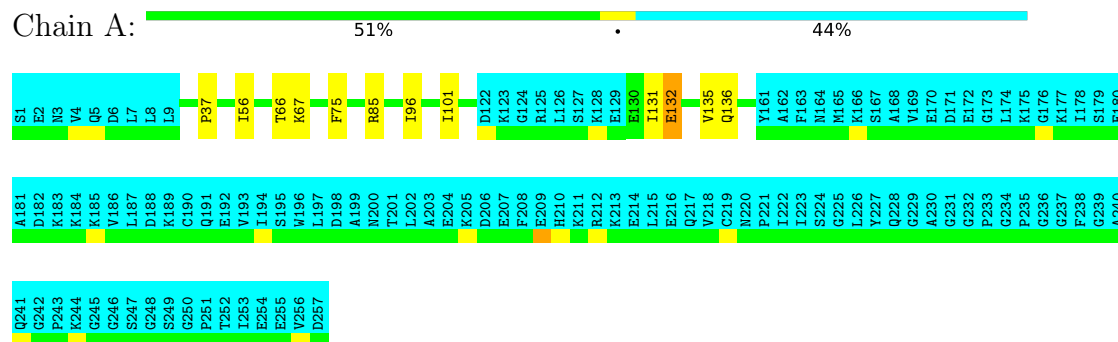
### 4.2.11 Score per residue for model 11

- Molecule 1: Heat shock 70 kDa protein 1A



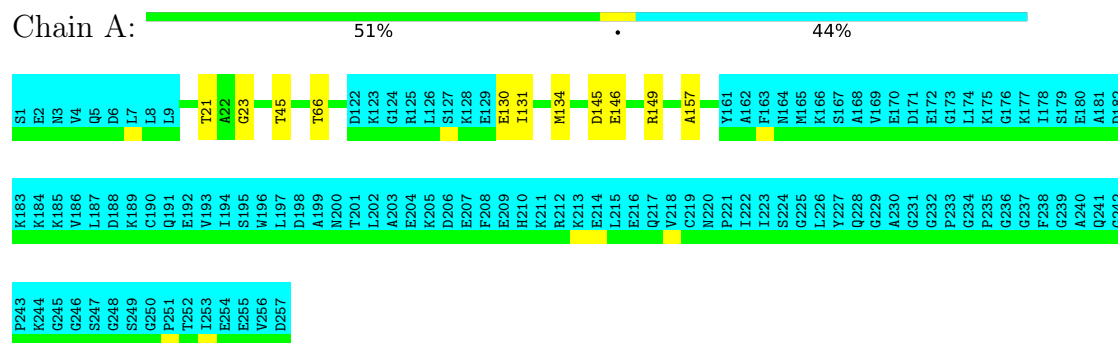
### 4.2.12 Score per residue for model 12

- Molecule 1: Heat shock 70 kDa protein 1A



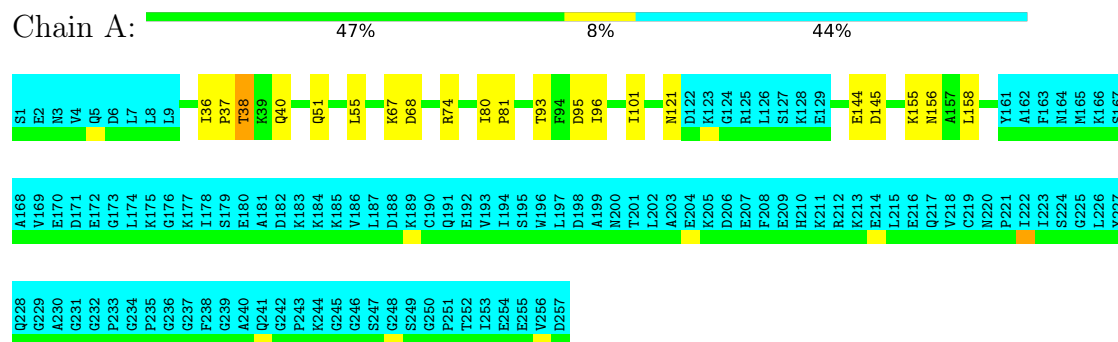
### 4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Heat shock 70 kDa protein 1A



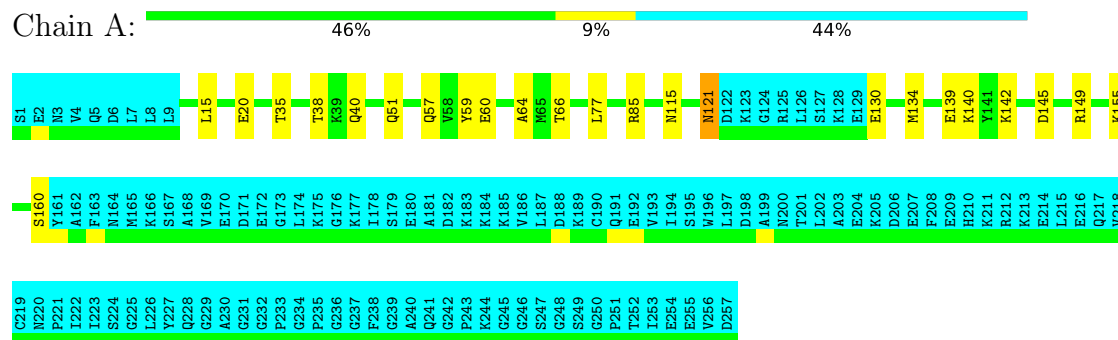
### 4.2.14 Score per residue for model 14

- Molecule 1: Heat shock 70 kDa protein 1A



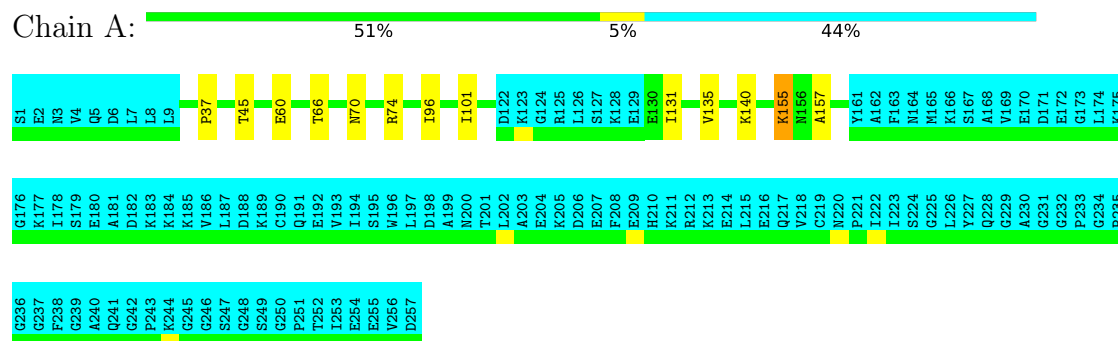
### 4.2.15 Score per residue for model 15

- Molecule 1: Heat shock 70 kDa protein 1A



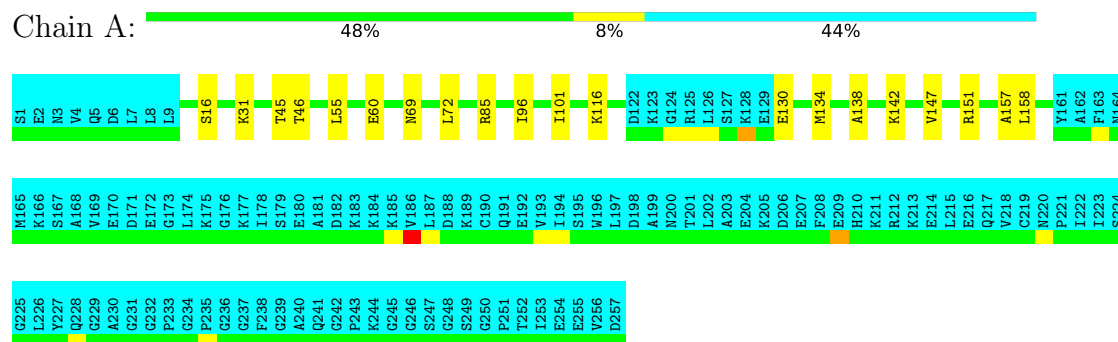
### 4.2.16 Score per residue for model 16

- Molecule 1: Heat shock 70 kDa protein 1A



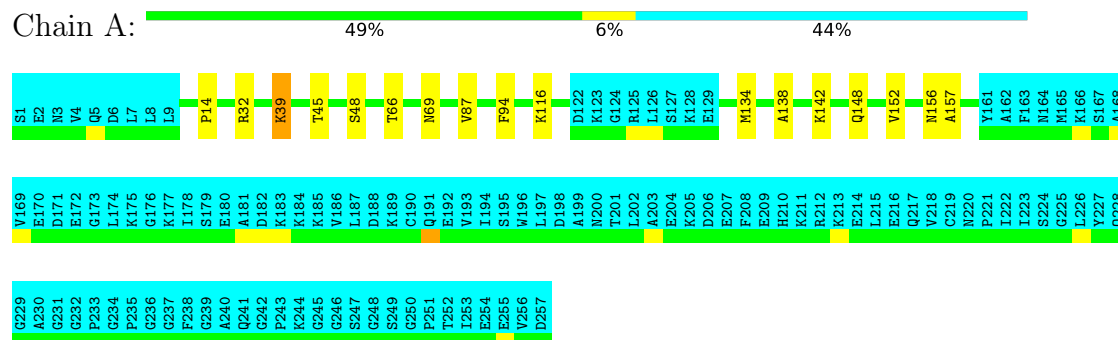
### 4.2.17 Score per residue for model 17

- Molecule 1: Heat shock 70 kDa protein 1A



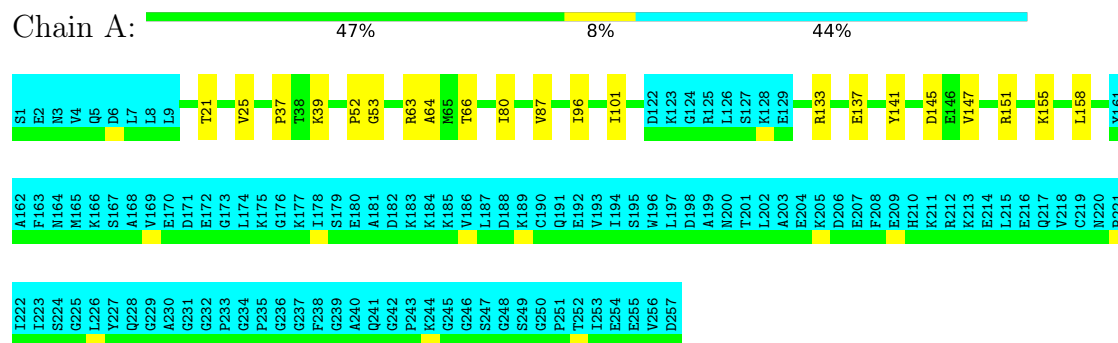
### 4.2.18 Score per residue for model 18

- Molecule 1: Heat shock 70 kDa protein 1A



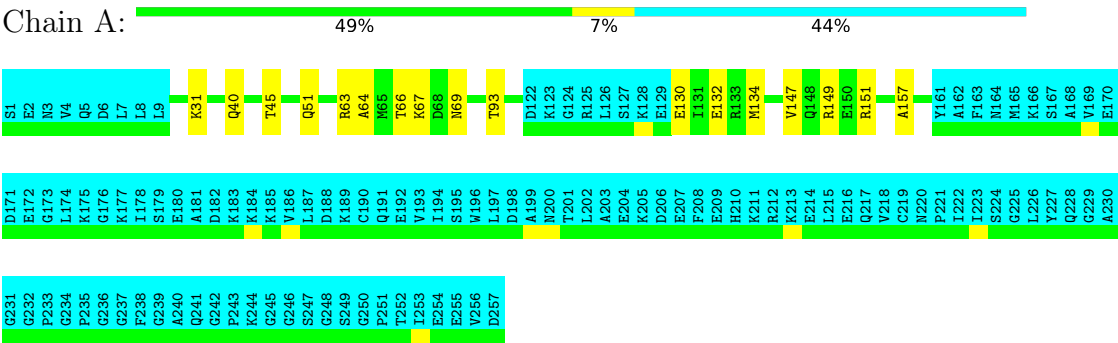
### 4.2.19 Score per residue for model 19

- Molecule 1: Heat shock 70 kDa protein 1A



4.2.20 Score per residue for model 20

- Molecule 1: Heat shock 70 kDa protein 1A



## 5 Refinement protocol and experimental data overview

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

Of the 50 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                       | 1851           |
| Number of shifts mapped to atoms             | 1851           |
| 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SMC

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     | 1.14±0.04    | 0±1/1107 ( 0.0± 0.1%) | 0.92±0.03   | 0±0/1501 ( 0.0± 0.0%) |
| All | All   | 1.14         | 8/22140 ( 0.0%)       | 0.92        | 5/30020 ( 0.0%)       |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 0.4±0.6   |
| All | All   | 0         | 8         |

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     | 66  | THR  | N-CA  | -5.91 | 1.39        | 1.46     | 19     | 1     |
| 1   | A     | 68  | ASP  | CA-C  | -5.64 | 1.46        | 1.53     | 14     | 1     |
| 1   | A     | 38  | THR  | N-CA  | -5.59 | 1.40        | 1.47     | 7      | 1     |
| 1   | A     | 87  | VAL  | CA-CB | 5.56  | 1.57        | 1.54     | 19     | 1     |
| 1   | A     | 81  | PRO  | CA-C  | 5.27  | 1.54        | 1.51     | 14     | 1     |
| 1   | A     | 53  | GLY  | N-CA  | -5.22 | 1.40        | 1.45     | 19     | 1     |
| 1   | A     | 48  | SER  | N-CA  | -5.18 | 1.40        | 1.46     | 18     | 1     |
| 1   | A     | 87  | VAL  | C-N   | 5.17  | 1.39        | 1.33     | 18     | 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( $^{\circ}$ ) | Ideal( $^{\circ}$ ) | Models |       |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|--------|-------|
|     |       |     |      |        |       |                        |                     | Worst  | Total |
| 1   | A     | 155 | LYS  | N-CA-C | -6.09 | 104.06                 | 112.03              | 4      | 1     |
| 1   | A     | 47  | TYR  | N-CA-C | -5.33 | 105.13                 | 111.69              | 1      | 2     |
| 1   | A     | 154 | ALA  | N-CA-C | -5.28 | 105.54                 | 112.41              | 6      | 1     |
| 1   | A     | 121 | ASN  | N-CA-C | -5.03 | 105.87                 | 111.36              | 14     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 63  | ARG  | Sidechain | 3              |
| 1   | A     | 74  | ARG  | Sidechain | 2              |
| 1   | A     | 32  | ARG  | Sidechain | 2              |
| 1   | A     | 149 | ARG  | Sidechain | 1              |

## 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes   |
|-----|-------|-------|----------|----------|-----------|
| 1   | A     | 1094  | 1109     | 1109     | 7 $\pm$ 2 |
| All | All   | 21880 | 22180    | 22180    | 135       |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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

| Atom-1         | Atom-2          | Clash( $\text{\AA}$ ) | Distance( $\text{\AA}$ ) | Models |       |
|----------------|-----------------|-----------------------|--------------------------|--------|-------|
|                |                 |                       |                          | Worst  | Total |
| 1:A:53:GLY:HA2 | 1:A:77:LEU:O    | 0.56                  | 2.00                     | 9      | 1     |
| 1:A:147:VAL:O  | 1:A:151:ARG:HG2 | 0.56                  | 2.01                     | 20     | 7     |
| 1:A:39:LYS:HA  | 1:A:94:PHE:O    | 0.54                  | 2.02                     | 18     | 1     |
| 1:A:62:GLU:OE2 | 1:A:67:LYS:HG3  | 0.54                  | 2.02                     | 11     | 1     |
| 1:A:130:GLU:O  | 1:A:134:MET:HG2 | 0.53                  | 2.03                     | 17     | 4     |
| 1:A:147:VAL:O  | 1:A:151:ARG:HG3 | 0.53                  | 2.02                     | 10     | 1     |
| 1:A:130:GLU:O  | 1:A:134:MET:HG3 | 0.53                  | 2.03                     | 15     | 2     |
| 1:A:45:THR:O   | 1:A:157:ALA:HA  | 0.53                  | 2.04                     | 3      | 11    |
| 1:A:21:THR:HB  | 1:A:157:ALA:O   | 0.52                  | 2.03                     | 13     | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:56:ILE:HB   | 1:A:75:PHE:HB3   | 0.52     | 1.81        | 12     | 1     |
| 1:A:96:ILE:HA   | 1:A:101:ILE:O    | 0.52     | 2.05        | 12     | 7     |
| 1:A:88:PRO:HA   | 1:A:110:SER:OG   | 0.51     | 2.05        | 6      | 1     |
| 1:A:29:LEU:HG   | 1:A:42:GLN:OE1   | 0.51     | 2.06        | 10     | 1     |
| 1:A:69:ASN:HA   | 1:A:134:MET:SD   | 0.50     | 2.45        | 8      | 2     |
| 1:A:19:LEU:HA   | 1:A:57:GLN:O     | 0.50     | 2.06        | 9      | 1     |
| 1:A:51:GLN:O    | 1:A:80:ILE:HB    | 0.49     | 2.06        | 2      | 2     |
| 1:A:21:THR:HG22 | 1:A:158:LEU:HD23 | 0.49     | 1.85        | 19     | 3     |
| 1:A:131:ILE:O   | 1:A:135:VAL:HG23 | 0.49     | 2.08        | 16     | 2     |
| 1:A:52:PRO:HA   | 1:A:80:ILE:O     | 0.49     | 2.07        | 19     | 2     |
| 1:A:63:ARG:HG2  | 1:A:69:ASN:ND2   | 0.48     | 2.23        | 20     | 1     |
| 1:A:11:ASP:O    | 1:A:35:THR:HA    | 0.48     | 2.09        | 3      | 3     |
| 1:A:59:TYR:HA   | 1:A:70:ASN:O     | 0.48     | 2.09        | 3      | 2     |
| 1:A:146:GLU:O   | 1:A:150:GLU:HG2  | 0.48     | 2.09        | 5      | 1     |
| 1:A:62:GLU:OE1  | 1:A:67:LYS:HG3   | 0.47     | 2.09        | 4      | 1     |
| 1:A:46:THR:O    | 1:A:85:ARG:HG2   | 0.47     | 2.09        | 17     | 1     |
| 1:A:138:ALA:O   | 1:A:142:LYS:HG2  | 0.47     | 2.10        | 18     | 2     |
| 1:A:132:GLU:O   | 1:A:136:GLN:HG2  | 0.47     | 2.10        | 12     | 1     |
| 1:A:63:ARG:HG3  | 1:A:67:LYS:O     | 0.47     | 2.10        | 20     | 2     |
| 1:A:142:LYS:O   | 1:A:146:GLU:HB2  | 0.47     | 2.09        | 4      | 1     |
| 1:A:32:ARG:H    | 1:A:32:ARG:HD3   | 0.47     | 1.70        | 1      | 1     |
| 1:A:130:GLU:H   | 1:A:130:GLU:CD   | 0.47     | 2.18        | 11     | 2     |
| 1:A:155:LYS:HA  | 1:A:155:LYS:HE3  | 0.46     | 1.87        | 16     | 1     |
| 1:A:47:TYR:O    | 1:A:85:ARG:HG2   | 0.45     | 2.11        | 2      | 1     |
| 1:A:40:GLN:O    | 1:A:93:THR:HA    | 0.45     | 2.12        | 20     | 3     |
| 1:A:139:GLU:O   | 1:A:142:LYS:HG2  | 0.45     | 2.10        | 15     | 1     |
| 1:A:64:ALA:HB2  | 1:A:145:ASP:O    | 0.45     | 2.12        | 19     | 2     |
| 1:A:136:GLN:O   | 1:A:140:LYS:HG3  | 0.45     | 2.12        | 4      | 1     |
| 1:A:146:GLU:O   | 1:A:149:ARG:HG2  | 0.45     | 2.11        | 8      | 1     |
| 1:A:77:LEU:HG   | 1:A:115:ASN:OD1  | 0.45     | 2.11        | 15     | 1     |
| 1:A:25:VAL:HA   | 1:A:64:ALA:O     | 0.45     | 2.12        | 19     | 1     |
| 1:A:60:GLU:CG   | 1:A:70:ASN:HB2   | 0.45     | 2.42        | 16     | 1     |
| 1:A:15:LEU:HB2  | 1:A:60:GLU:CG    | 0.44     | 2.43        | 10     | 2     |
| 1:A:142:LYS:HA  | 1:A:142:LYS:HE3  | 0.44     | 1.89        | 10     | 1     |
| 1:A:40:GLN:HE22 | 1:A:42:GLN:HG3   | 0.44     | 1.73        | 3      | 1     |
| 1:A:36:ILE:HB   | 1:A:37:PRO:HA    | 0.44     | 1.90        | 14     | 1     |
| 1:A:12:VAL:HA   | 1:A:34:SER:O     | 0.44     | 2.13        | 8      | 1     |
| 1:A:37:PRO:HA   | 1:A:96:ILE:O     | 0.44     | 2.12        | 16     | 3     |
| 1:A:142:LYS:HA  | 1:A:142:LYS:CE   | 0.44     | 2.43        | 10     | 1     |
| 1:A:145:ASP:O   | 1:A:149:ARG:HG2  | 0.43     | 2.13        | 13     | 1     |
| 1:A:16:SER:HB2  | 1:A:62:GLU:HG3   | 0.43     | 1.91        | 10     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:148:GLN:O   | 1:A:152:VAL:HG23 | 0.43     | 2.13        | 18     | 1     |
| 1:A:133:ARG:O   | 1:A:137:GLU:HG2  | 0.43     | 2.13        | 19     | 1     |
| 1:A:159:GLU:CD  | 1:A:160:SER:H    | 0.43     | 2.22        | 3      | 1     |
| 1:A:64:ALA:HB2  | 1:A:145:ASP:HA   | 0.43     | 1.90        | 5      | 2     |
| 1:A:36:ILE:HA   | 1:A:37:PRO:C     | 0.43     | 2.38        | 7      | 5     |
| 1:A:141:TYR:HB3 | 1:A:145:ASP:OD1  | 0.43     | 2.14        | 19     | 1     |
| 1:A:20:GLU:HB2  | 1:A:59:TYR:CE2   | 0.42     | 2.49        | 15     | 1     |
| 1:A:138:ALA:O   | 1:A:142:LYS:HB3  | 0.42     | 2.14        | 17     | 1     |
| 1:A:22:ALA:HB2  | 1:A:47:TYR:CE2   | 0.42     | 2.49        | 8      | 1     |
| 1:A:38:THR:O    | 1:A:95:ASP:HA    | 0.42     | 2.13        | 14     | 1     |
| 1:A:39:LYS:HD2  | 1:A:95:ASP:HB3   | 0.42     | 1.90        | 4      | 1     |
| 1:A:135:VAL:O   | 1:A:139:GLU:HG2  | 0.42     | 2.14        | 4      | 1     |
| 1:A:104:VAL:O   | 1:A:116:LYS:HA   | 0.42     | 2.15        | 10     | 2     |
| 1:A:47:TYR:CD1  | 1:A:157:ALA:HB2  | 0.42     | 2.50        | 10     | 1     |
| 1:A:16:SER:O    | 1:A:60:GLU:HB2   | 0.42     | 2.13        | 17     | 1     |
| 1:A:14:PRO:O    | 1:A:32:ARG:HD2   | 0.42     | 2.15        | 18     | 1     |
| 1:A:144:GLU:O   | 1:A:148:GLN:HG2  | 0.41     | 2.15        | 2      | 1     |
| 1:A:44:PHE:HA   | 1:A:156:ASN:ND2  | 0.41     | 2.30        | 10     | 1     |
| 1:A:11:ASP:O    | 1:A:36:ILE:HG12  | 0.41     | 2.14        | 11     | 1     |
| 1:A:16:SER:HA   | 1:A:30:ILE:O     | 0.41     | 2.15        | 4      | 1     |
| 1:A:155:LYS:HA  | 1:A:155:LYS:CE   | 0.41     | 2.45        | 16     | 1     |
| 1:A:63:ARG:O    | 1:A:149:ARG:HD3  | 0.41     | 2.16        | 6      | 1     |
| 1:A:85:ARG:C    | 1:A:85:ARG:HD3   | 0.41     | 2.40        | 17     | 1     |
| 1:A:146:GLU:OE1 | 1:A:149:ARG:HD3  | 0.41     | 2.15        | 13     | 1     |
| 1:A:60:GLU:O    | 1:A:69:ASN:HB3   | 0.41     | 2.15        | 1      | 1     |
| 1:A:51:GLN:NE2  | 1:A:160:SER:HB2  | 0.41     | 2.31        | 15     | 1     |
| 1:A:132:GLU:O   | 1:A:136:GLN:HG3  | 0.41     | 2.16        | 5      | 1     |
| 1:A:29:LEU:HA   | 1:A:42:GLN:NE2   | 0.41     | 2.31        | 5      | 1     |
| 1:A:134:MET:HA  | 1:A:134:MET:HE3  | 0.40     | 1.93        | 3      | 1     |
| 1:A:38:THR:OG1  | 1:A:96:ILE:HB    | 0.40     | 2.16        | 14     | 1     |
| 1:A:74:ARG:O    | 1:A:74:ARG:HD2   | 0.40     | 2.17        | 3      | 1     |
| 1:A:64:ALA:HA   | 1:A:149:ARG:HB2  | 0.40     | 1.91        | 20     | 1     |
| 1:A:149:ARG:HD3 | 1:A:149:ARG:C    | 0.40     | 2.42        | 2      | 1     |
| 1:A:55:LEU:HD21 | 1:A:74:ARG:NH1   | 0.40     | 2.32        | 14     | 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     | 143/257 (56%)   | 133±3 (93±2%) | 9±3 (6±2%) | 2±1 (1±1%) | 14          | 63 |
| All | All   | 2860/5140 (56%) | 2653 (93%)    | 175 (6%)   | 32 (1%)    | 14          | 63 |

All 17 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     | 67  | LYS  | 5              |
| 1   | A     | 85  | ARG  | 3              |
| 1   | A     | 39  | LYS  | 3              |
| 1   | A     | 121 | ASN  | 3              |
| 1   | A     | 23  | GLY  | 2              |
| 1   | A     | 154 | ALA  | 2              |
| 1   | A     | 79  | GLY  | 2              |
| 1   | A     | 155 | LYS  | 2              |
| 1   | A     | 156 | ASN  | 2              |
| 1   | A     | 24  | GLY  | 1              |
| 1   | A     | 50  | ASN  | 1              |
| 1   | A     | 62  | GLU  | 1              |
| 1   | A     | 63  | ARG  | 1              |
| 1   | A     | 84  | PRO  | 1              |
| 1   | A     | 10  | LEU  | 1              |
| 1   | A     | 87  | VAL  | 1              |
| 1   | A     | 69  | ASN  | 1              |

### 6.3.2 Protein sidechains ⓘ

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     | 121/210 (58%)   | 117±2 (97±1%) | 4±2 (3±1%) | 37          | 85 |
| All | All   | 2420/4200 (58%) | 2347 (97%)    | 73 (3%)    | 37          | 85 |

All 32 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     | 66  | THR  | 16             |
| 1   | A     | 38  | THR  | 5              |
| 1   | A     | 35  | THR  | 4              |
| 1   | A     | 145 | ASP  | 4              |
| 1   | A     | 40  | GLN  | 3              |
| 1   | A     | 51  | GLN  | 3              |
| 1   | A     | 31  | LYS  | 3              |
| 1   | A     | 20  | GLU  | 2              |
| 1   | A     | 32  | ARG  | 2              |
| 1   | A     | 39  | LYS  | 2              |
| 1   | A     | 159 | GLU  | 2              |
| 1   | A     | 60  | GLU  | 2              |
| 1   | A     | 144 | GLU  | 2              |
| 1   | A     | 158 | LEU  | 2              |
| 1   | A     | 140 | LYS  | 2              |
| 1   | A     | 155 | LYS  | 2              |
| 1   | A     | 116 | LYS  | 2              |
| 1   | A     | 42  | GLN  | 1              |
| 1   | A     | 89  | GLN  | 1              |
| 1   | A     | 67  | LYS  | 1              |
| 1   | A     | 90  | ILE  | 1              |
| 1   | A     | 133 | ARG  | 1              |
| 1   | A     | 80  | ILE  | 1              |
| 1   | A     | 142 | LYS  | 1              |
| 1   | A     | 85  | ARG  | 1              |
| 1   | A     | 132 | GLU  | 1              |
| 1   | A     | 57  | GLN  | 1              |
| 1   | A     | 121 | ASN  | 1              |
| 1   | A     | 149 | ARG  | 1              |
| 1   | A     | 74  | ARG  | 1              |
| 1   | A     | 55  | LEU  | 1              |
| 1   | A     | 72  | LEU  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds

that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 1   | SMC  | A     | 219 | 1    | 4,5,7        | 1.06±0.21 | 0±0 (2±7%) |
| 1   | SMC  | A     | 190 | 1    | 4,5,7        | 1.00±0.21 | 0±0 (0±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 1   | SMC  | A     | 219 | 1    | 1,5,8       | 0.20±0.16 | 0±0 (0±0%) |
| 1   | SMC  | A     | 190 | 1    | 1,5,8       | 0.23±0.18 | 0±0 (0±0%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 1   | SMC  | A     | 190 | 1    | -       | 0±0,1,4,7 | -     |
| 1   | SMC  | A     | 219 | 1    | -       | 0±0,1,4,7 | -     |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 219 | SMC  | CB-CA | 2.53 | 1.55        | 1.53     | 12     | 2     |

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 55% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1851 |
| Number of shifts mapped to atoms        | 1851 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 1    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 165      | $-0.20 \pm 0.10$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 148      | $-0.07 \pm 0.13$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 157      | $0.16 \pm 0.05$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 149      | $-0.21 \pm 0.20$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1586 atoms were assigned a chemical shift out of a possible 1913. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 679/711 (95%)  | 278/289 (96%) | 271/286 (95%)   | 130/136 (96%)   |
| Sidechain | 893/1145 (78%) | 597/742 (80%) | 289/357 (81%)   | 7/46 (15%)      |

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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 | 14/57 (25%)     | 9/27 (33%)           | 5/30 (17%)            | 0/0 (—%)              |
| Overall  | 1586/1913 (83%) | 884/1058 (84%)       | 565/673 (84%)         | 137/182 (75%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 1851 atoms were assigned a chemical shift out of a possible 3348. 0 out of 37 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  | 791/1277 (62%)  | 320/524 (61%)        | 322/510 (63%)         | 149/243 (61%)         |
| Sidechain | 1040/1946 (53%) | 692/1255 (55%)       | 341/617 (55%)         | 7/74 (9%)             |
| Aromatic  | 20/125 (16%)    | 12/60 (20%)          | 7/62 (11%)            | 1/3 (33%)             |
| Overall   | 1851/3348 (55%) | 1024/1839 (56%)      | 670/1189 (56%)        | 157/320 (49%)         |

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

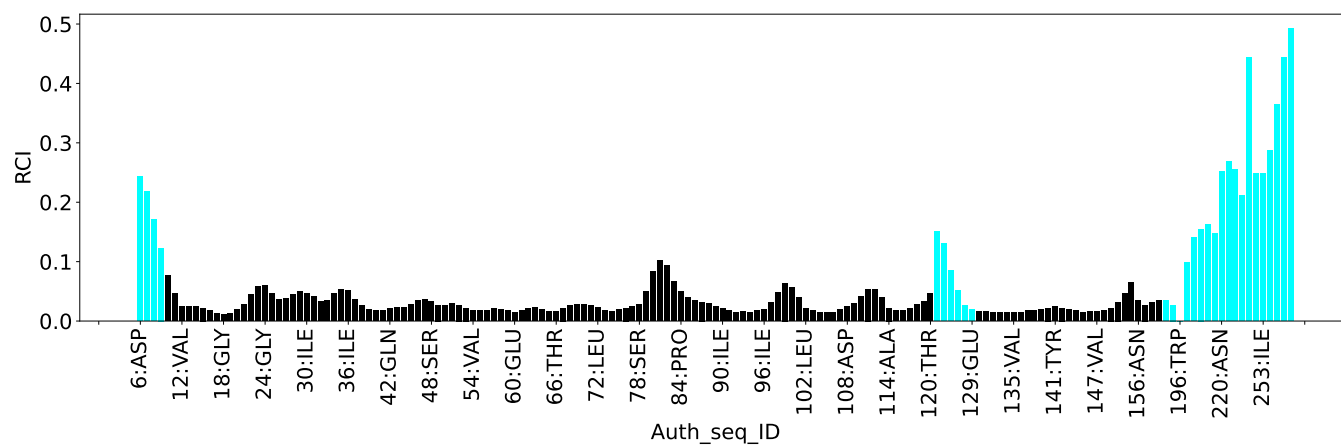
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 66  | THR  | HB   | 2.23       | 2.57 – 5.77         | -6.0    |

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

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

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 3291  |
| Intra-residue ( $ i-j =0$ )                              | 1108  |
| Sequential ( $ i-j =1$ )                                 | 716   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 391   |
| Long range ( $ i-j \geq 5$ )                             | 986   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 90    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 257   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 13.8  |
| Number of long range restraints per residue <sup>1</sup> | 4.1   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 25.2                                   | 0.2     |
| 0.2-0.5 (Medium) | 42.5                                   | 0.5     |
| >0.5 (Large)     | 35.6                                   | 2.23    |

### 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)   | 9.8                                    | 3.68    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

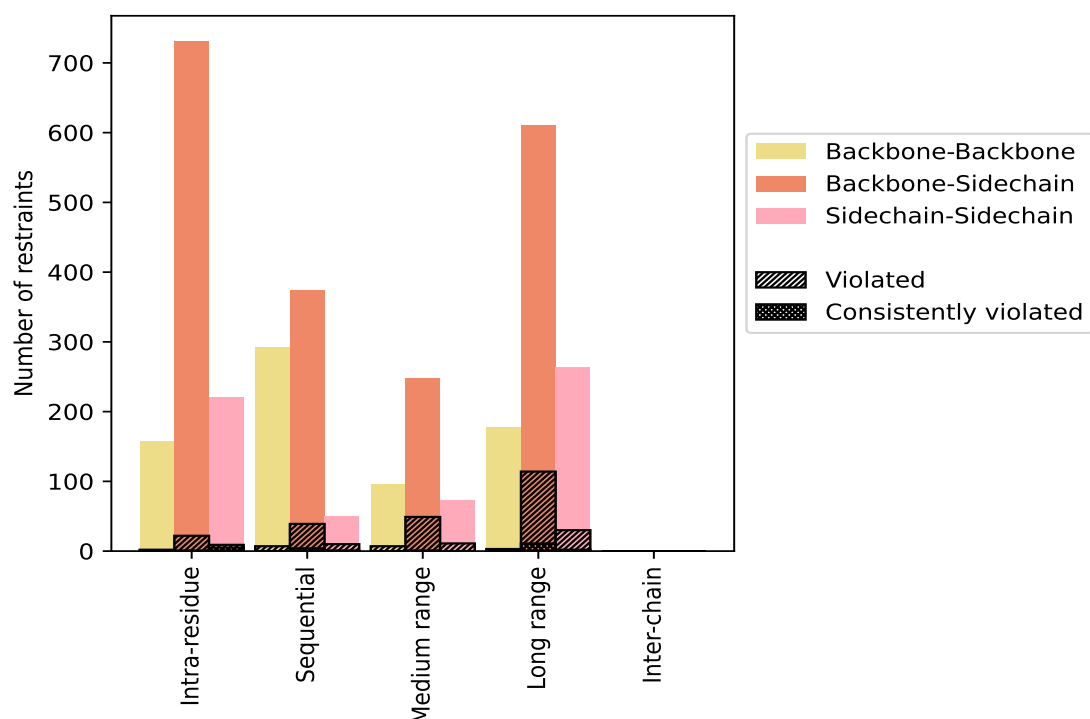
### 9.1 Summary of distance violations ⓘ

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>1108</b> | <b>33.7</b>    | <b>33</b>             | <b>3.0</b>     | <b>1.0</b>     | <b>6</b>                           | <b>0.5</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 157         | 4.8            | 2                     | 1.3            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 731         | 22.2           | 22                    | 3.0            | 0.7            | 1                                  | 0.1            | 0.0            |
| Sidechain-Sidechain                                                         | 220         | 6.7            | 9                     | 4.1            | 0.3            | 5                                  | 2.3            | 0.2            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>716</b>  | <b>21.8</b>    | <b>56</b>             | <b>7.8</b>     | <b>1.7</b>     | <b>5</b>                           | <b>0.7</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 292         | 8.9            | 7                     | 2.4            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 374         | 11.4           | 39                    | 10.4           | 1.2            | 4                                  | 1.1            | 0.1            |
| Sidechain-Sidechain                                                         | 50          | 1.5            | 10                    | 20.0           | 0.3            | 1                                  | 2.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>391</b>  | <b>11.9</b>    | <b>67</b>             | <b>17.1</b>    | <b>2.0</b>     | <b>1</b>                           | <b>0.3</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 96          | 2.9            | 7                     | 7.3            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 223         | 6.8            | 49                    | 22.0           | 1.5            | 1                                  | 0.4            | 0.0            |
| Sidechain-Sidechain                                                         | 72          | 2.2            | 11                    | 15.3           | 0.3            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>986</b>  | <b>30.0</b>    | <b>146</b>            | <b>14.8</b>    | <b>4.4</b>     | <b>13</b>                          | <b>1.3</b>     | <b>0.4</b>     |
| Backbone-Backbone                                                           | 178         | 5.4            | 3                     | 1.7            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 544         | 16.5           | 113                   | 20.8           | 3.4            | 11                                 | 2.0            | 0.3            |
| Sidechain-Sidechain                                                         | 264         | 8.0            | 30                    | 11.4           | 0.9            | 2                                  | 0.8            | 0.1            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>90</b>   | <b>2.7</b>     | <b>1</b>              | <b>1.1</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>3291</b> | <b>100.0</b>   | <b>303</b>            | <b>9.2</b>     | <b>9.2</b>     | <b>25</b>                          | <b>0.8</b>     | <b>0.8</b>     |
| Backbone-Backbone                                                           | 723         | 22.0           | 19                    | 2.6            | 0.6            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1962        | 59.6           | 224                   | 11.4           | 6.8            | 17                                 | 0.9            | 0.5            |
| Sidechain-Sidechain                                                         | 606         | 18.4           | 60                    | 9.9            | 1.8            | 8                                  | 1.3            | 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        | 22                   | 32              | 16              | 49              | 0               | 119   | 0.48     | 2.23    | 0.37                | 0.35       |
| 2        | 20                   | 28              | 15              | 47              | 0               | 110   | 0.45     | 1.98    | 0.35                | 0.33       |
| 3        | 18                   | 24              | 20              | 39              | 0               | 101   | 0.42     | 1.62    | 0.31                | 0.31       |
| 4        | 23                   | 25              | 15              | 44              | 0               | 107   | 0.47     | 1.54    | 0.33                | 0.38       |
| 5        | 17                   | 31              | 12              | 43              | 0               | 103   | 0.46     | 1.55    | 0.32                | 0.39       |
| 6        | 16                   | 28              | 16              | 35              | 0               | 95    | 0.49     | 1.52    | 0.35                | 0.39       |
| 7        | 21                   | 28              | 9               | 43              | 0               | 101   | 0.44     | 1.48    | 0.31                | 0.34       |
| 8        | 22                   | 25              | 14              | 42              | 0               | 103   | 0.49     | 1.46    | 0.32                | 0.4        |
| 9        | 19                   | 23              | 15              | 42              | 0               | 99    | 0.46     | 1.55    | 0.32                | 0.38       |
| 10       | 19                   | 27              | 17              | 35              | 0               | 98    | 0.48     | 1.48    | 0.32                | 0.34       |

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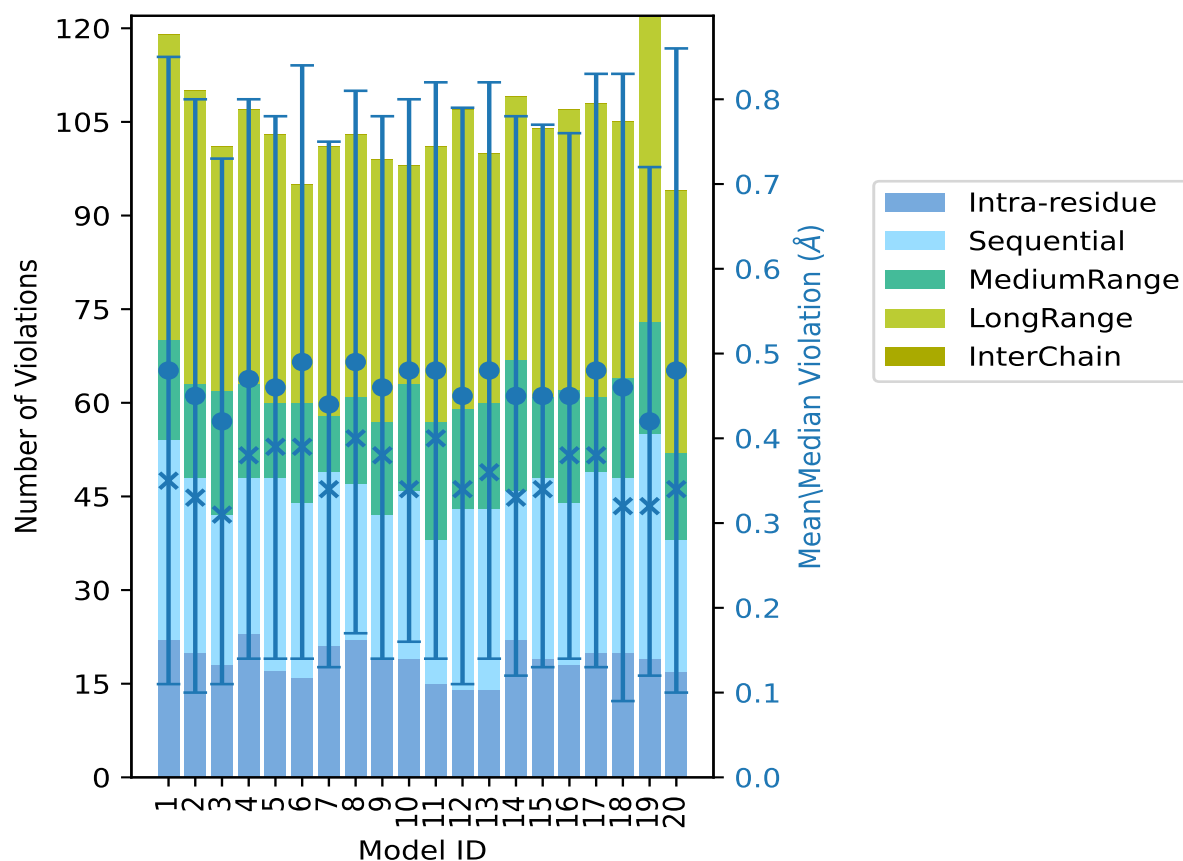
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 15                   | 23              | 19              | 44              | 0               | 101   | 0.48     | 1.61    | 0.34                | 0.4        |
| 12       | 14                   | 29              | 16              | 48              | 0               | 107   | 0.45     | 1.53    | 0.34                | 0.34       |
| 13       | 14                   | 29              | 17              | 40              | 0               | 100   | 0.48     | 1.56    | 0.34                | 0.36       |
| 14       | 22                   | 24              | 21              | 42              | 0               | 109   | 0.45     | 1.6     | 0.33                | 0.33       |
| 15       | 19                   | 29              | 13              | 43              | 0               | 104   | 0.45     | 1.45    | 0.32                | 0.34       |
| 16       | 18                   | 26              | 18              | 45              | 0               | 107   | 0.45     | 1.95    | 0.31                | 0.38       |
| 17       | 20                   | 29              | 12              | 47              | 0               | 108   | 0.48     | 1.75    | 0.35                | 0.38       |
| 18       | 20                   | 28              | 16              | 41              | 0               | 105   | 0.46     | 1.57    | 0.37                | 0.32       |
| 19       | 19                   | 36              | 18              | 49              | 0               | 122   | 0.42     | 1.33    | 0.3                 | 0.32       |
| 20       | 17                   | 21              | 14              | 42              | 0               | 94    | 0.48     | 1.7     | 0.38                | 0.34       |

<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

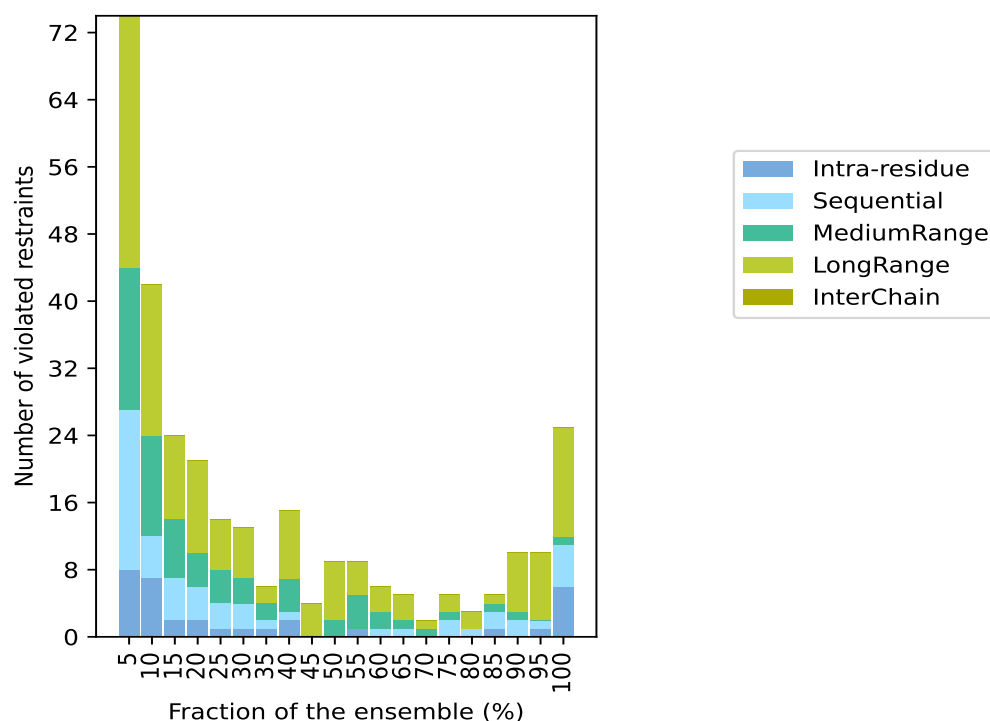
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2899(IR:1075, SQ:660, MR:324, LR:840, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 8                             | 19              | 17              | 30              | 0               | 74    | 1                        | 5.0   |
| 7                             | 5               | 12              | 18              | 0               | 42    | 2                        | 10.0  |
| 2                             | 5               | 7               | 10              | 0               | 24    | 3                        | 15.0  |
| 2                             | 4               | 4               | 11              | 0               | 21    | 4                        | 20.0  |
| 1                             | 3               | 4               | 6               | 0               | 14    | 5                        | 25.0  |
| 1                             | 3               | 3               | 6               | 0               | 13    | 6                        | 30.0  |
| 1                             | 1               | 2               | 2               | 0               | 6     | 7                        | 35.0  |
| 2                             | 1               | 4               | 8               | 0               | 15    | 8                        | 40.0  |
| 0                             | 0               | 0               | 4               | 0               | 4     | 9                        | 45.0  |
| 0                             | 0               | 2               | 7               | 0               | 9     | 10                       | 50.0  |
| 1                             | 0               | 4               | 4               | 0               | 9     | 11                       | 55.0  |
| 0                             | 1               | 2               | 3               | 0               | 6     | 12                       | 60.0  |
| 0                             | 1               | 1               | 3               | 0               | 5     | 13                       | 65.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 14                       | 70.0  |
| 0                             | 2               | 1               | 2               | 0               | 5     | 15                       | 75.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 16                       | 80.0  |
| 1                             | 2               | 1               | 1               | 0               | 5     | 17                       | 85.0  |
| 0                             | 2               | 1               | 7               | 0               | 10    | 18                       | 90.0  |
| 1                             | 1               | 0               | 8               | 0               | 10    | 19                       | 95.0  |
| 6                             | 5               | 1               | 13              | 0               | 25    | 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

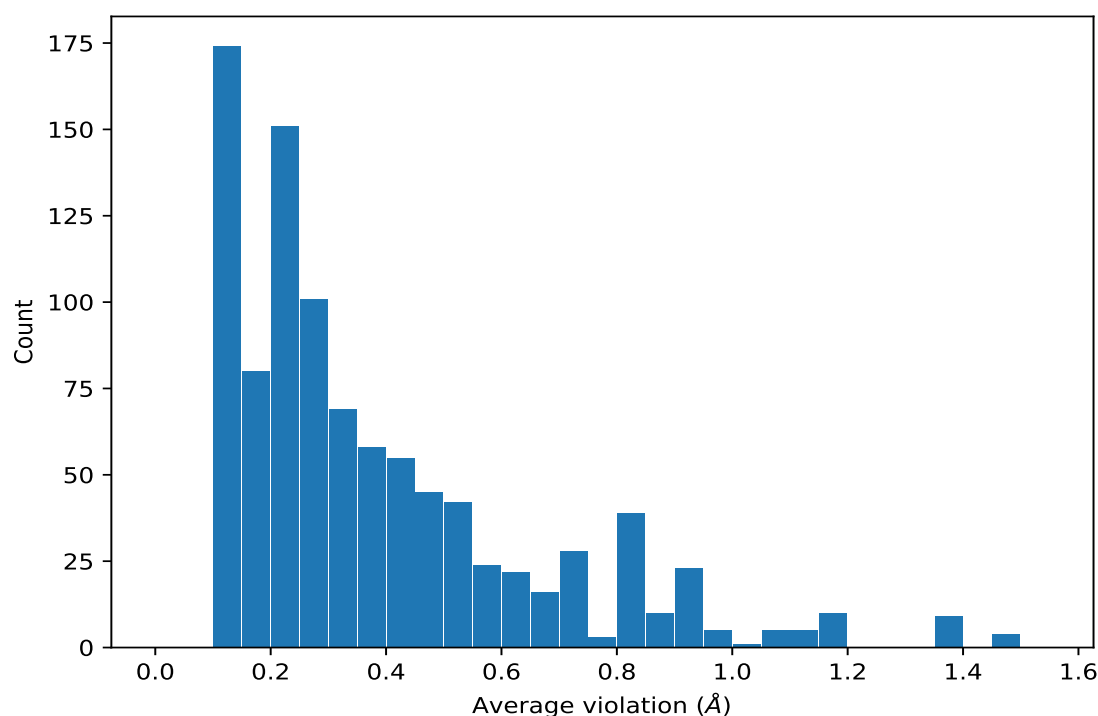
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2159) | 1:36:A:ILE:HG23 | 1:37:A:PRO:HD3  | 20                  | 1.49     | 0.09                | 1.52       |
| (1,2159) | 1:36:A:ILE:HG21 | 1:37:A:PRO:HD3  | 20                  | 1.49     | 0.09                | 1.52       |
| (1,2159) | 1:36:A:ILE:HG22 | 1:37:A:PRO:HD3  | 20                  | 1.49     | 0.09                | 1.52       |
| (1,2159) | 1:36:A:ILE:HG22 | 1:32:A:ARG:HA   | 20                  | 1.49     | 0.09                | 1.52       |
| (1,2481) | 1:103:A:ASN:H   | 1:30:A:ILE:HD13 | 20                  | 1.17     | 0.23                | 1.19       |
| (1,2481) | 1:103:A:ASN:H   | 1:96:A:ILE:HD12 | 20                  | 1.17     | 0.23                | 1.19       |
| (1,2481) | 1:103:A:ASN:H   | 1:96:A:ILE:HD13 | 20                  | 1.17     | 0.23                | 1.19       |
| (1,2481) | 1:103:A:ASN:H   | 1:30:A:ILE:HD11 | 20                  | 1.17     | 0.23                | 1.19       |
| (1,2481) | 1:103:A:ASN:H   | 1:30:A:ILE:HD12 | 20                  | 1.17     | 0.23                | 1.19       |
| (1,2481) | 1:103:A:ASN:H   | 1:96:A:ILE:HD11 | 20                  | 1.17     | 0.23                | 1.19       |
| (1,3193) | 1:35:A:THR:H    | 1:12:A:VAL:HG22 | 20                  | 1.16     | 0.11                | 1.18       |
| (1,3193) | 1:35:A:THR:H    | 1:36:A:ILE:HG12 | 20                  | 1.16     | 0.11                | 1.18       |
| (1,3193) | 1:35:A:THR:H    | 1:12:A:VAL:HG21 | 20                  | 1.16     | 0.11                | 1.18       |
| (1,3193) | 1:35:A:THR:H    | 1:12:A:VAL:HG23 | 20                  | 1.16     | 0.11                | 1.18       |
| (1,3154) | 1:46:A:THR:H    | 1:80:A:ILE:HG21 | 20                  | 1.11     | 0.32                | 1.16       |
| (1,3154) | 1:46:A:THR:H    | 1:80:A:ILE:HG23 | 20                  | 1.11     | 0.32                | 1.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3154) | 1:46:A:THR:H     | 1:87:A:VAL:HG23  | 20                  | 1.11     | 0.32                | 1.16       |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 20                  | 1.11     | 0.32                | 1.16       |
| (1,3154) | 1:46:A:THR:H     | 1:87:A:VAL:HG21  | 20                  | 1.11     | 0.32                | 1.16       |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD21  | 20                  | 1.09     | 0.26                | 1.12       |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD12  | 20                  | 1.09     | 0.26                | 1.12       |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD13  | 20                  | 1.09     | 0.26                | 1.12       |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD11  | 20                  | 1.09     | 0.26                | 1.12       |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD23  | 20                  | 1.09     | 0.26                | 1.12       |
| (1,3028) | 1:59:A:TYR:H     | 1:60:A:GLU:HG3   | 20                  | 0.81     | 0.22                | 0.85       |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 20                  | 0.81     | 0.22                | 0.85       |
| (1,3028) | 1:59:A:TYR:H     | 1:60:A:GLU:HG2   | 20                  | 0.81     | 0.22                | 0.85       |
| (1,3028) | 1:59:A:TYR:H     | 1:26:A:MET:HB2   | 20                  | 0.81     | 0.22                | 0.85       |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG22 | 20                  | 0.81     | 0.19                | 0.89       |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD12 | 20                  | 0.81     | 0.19                | 0.89       |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG21 | 20                  | 0.81     | 0.19                | 0.89       |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD21 | 20                  | 0.81     | 0.19                | 0.89       |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD22 | 20                  | 0.81     | 0.19                | 0.89       |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG23 | 20                  | 0.81     | 0.19                | 0.89       |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD11  | 20                  | 0.8      | 0.16                | 0.83       |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD13  | 20                  | 0.8      | 0.16                | 0.83       |
| (1,3150) | 1:96:A:ILE:HB    | 1:102:A:LEU:HD11 | 20                  | 0.8      | 0.16                | 0.83       |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD12  | 20                  | 0.8      | 0.16                | 0.83       |
| (1,3150) | 1:96:A:ILE:HB    | 1:102:A:LEU:HD12 | 20                  | 0.8      | 0.16                | 0.83       |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 20                  | 0.77     | 0.3                 | 0.79       |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG12  | 20                  | 0.77     | 0.3                 | 0.79       |
| (1,2684) | 1:158:A:LEU:H    | 1:45:A:THR:HG23  | 20                  | 0.77     | 0.3                 | 0.79       |
| (1,3079) | 1:41:A:THR:HG23  | 1:41:A:THR:H     | 20                  | 0.74     | 0.18                | 0.77       |
| (1,3079) | 1:93:A:THR:HG22  | 1:41:A:THR:H     | 20                  | 0.74     | 0.18                | 0.77       |
| (1,3079) | 1:93:A:THR:HG21  | 1:41:A:THR:H     | 20                  | 0.74     | 0.18                | 0.77       |
| (1,3079) | 1:41:A:THR:HG21  | 1:41:A:THR:H     | 20                  | 0.74     | 0.18                | 0.77       |
| (1,3079) | 1:105:A:THR:HG21 | 1:105:A:THR:H    | 20                  | 0.74     | 0.18                | 0.77       |
| (1,3079) | 1:93:A:THR:HG22  | 1:105:A:THR:H    | 20                  | 0.74     | 0.18                | 0.77       |
| (1,3079) | 1:93:A:THR:HG23  | 1:41:A:THR:H     | 20                  | 0.74     | 0.18                | 0.77       |
| (1,3079) | 1:93:A:THR:HG21  | 1:105:A:THR:H    | 20                  | 0.74     | 0.18                | 0.77       |
| (1,1956) | 1:96:A:ILE:HD12  | 1:97:A:ASP:H     | 20                  | 0.73     | 0.14                | 0.73       |
| (1,1956) | 1:96:A:ILE:HD11  | 1:97:A:ASP:H     | 20                  | 0.73     | 0.14                | 0.73       |
| (1,1956) | 1:96:A:ILE:HD13  | 1:97:A:ASP:H     | 20                  | 0.73     | 0.14                | 0.73       |
| (1,3141) | 1:13:A:ALA:HB3   | 1:12:A:VAL:HB    | 20                  | 0.67     | 0.15                | 0.66       |
| (1,3141) | 1:13:A:ALA:HB2   | 1:32:A:ARG:HB2   | 20                  | 0.67     | 0.15                | 0.66       |
| (1,3141) | 1:13:A:ALA:HB2   | 1:12:A:VAL:HB    | 20                  | 0.67     | 0.15                | 0.66       |
| (1,3141) | 1:13:A:ALA:HB1   | 1:12:A:VAL:HB    | 20                  | 0.67     | 0.15                | 0.66       |
| (1,3141) | 1:13:A:ALA:HB3   | 1:32:A:ARG:HB3   | 20                  | 0.67     | 0.15                | 0.66       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3141) | 1:13:A:ALA:HB1   | 1:32:A:ARG:HB2   | 20                  | 0.67     | 0.15                | 0.66       |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD13 | 20                  | 0.54     | 0.15                | 0.54       |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD21 | 20                  | 0.54     | 0.15                | 0.54       |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD23 | 20                  | 0.54     | 0.15                | 0.54       |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD22 | 20                  | 0.54     | 0.15                | 0.54       |
| (1,2699) | 1:127:A:SER:H    | 1:131:A:ILE:HD11 | 20                  | 0.54     | 0.15                | 0.54       |
| (1,2699) | 1:127:A:SER:H    | 1:131:A:ILE:HD12 | 20                  | 0.54     | 0.15                | 0.54       |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD12 | 20                  | 0.54     | 0.15                | 0.54       |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD11 | 20                  | 0.54     | 0.15                | 0.54       |
| (1,2380) | 1:104:A:VAL:HG13 | 1:105:A:THR:HB   | 20                  | 0.5      | 0.09                | 0.48       |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 20                  | 0.5      | 0.09                | 0.48       |
| (1,2380) | 1:104:A:VAL:HG11 | 1:105:A:THR:HB   | 20                  | 0.5      | 0.09                | 0.48       |
| (1,2380) | 1:104:A:VAL:HG12 | 1:93:A:THR:HB    | 20                  | 0.5      | 0.09                | 0.48       |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 20                  | 0.45     | 0.07                | 0.46       |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 20                  | 0.45     | 0.07                | 0.46       |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG22 | 20                  | 0.45     | 0.07                | 0.46       |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG22 | 20                  | 0.43     | 0.12                | 0.42       |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG23 | 20                  | 0.43     | 0.12                | 0.42       |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG21 | 20                  | 0.43     | 0.12                | 0.42       |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG21  | 20                  | 0.37     | 0.15                | 0.33       |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG23  | 20                  | 0.37     | 0.15                | 0.33       |
| (1,2725) | 1:38:A:THR:H     | 1:96:A:ILE:HG13  | 20                  | 0.37     | 0.15                | 0.33       |
| (1,2725) | 1:38:A:THR:H     | 1:96:A:ILE:HG22  | 20                  | 0.37     | 0.15                | 0.33       |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG22  | 20                  | 0.37     | 0.15                | 0.33       |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 20                  | 0.34     | 0.03                | 0.33       |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG23 | 20                  | 0.34     | 0.03                | 0.33       |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG22 | 20                  | 0.34     | 0.03                | 0.33       |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG23  | 20                  | 0.3      | 0.11                | 0.26       |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22  | 20                  | 0.3      | 0.11                | 0.26       |
| (1,3192) | 1:13:A:ALA:H     | 1:36:A:ILE:HG12  | 20                  | 0.3      | 0.11                | 0.26       |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG21  | 20                  | 0.3      | 0.11                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD11  | 1:55:A:LEU:HB2   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD11  | 1:55:A:LEU:HB2   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD11  | 1:55:A:LEU:HB3   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD11  | 1:55:A:LEU:HB3   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD11  | 1:55:A:LEU:HB2   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD11  | 1:55:A:LEU:HB2   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD11  | 1:55:A:LEU:HB3   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD11  | 1:55:A:LEU:HB3   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD12  | 1:55:A:LEU:HB2   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD12  | 1:55:A:LEU:HB2   | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD12  | 1:55:A:LEU:HB3   | 20                  | 0.25     | 0.03                | 0.26       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 20                  | 0.25     | 0.03                | 0.26       |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |

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| Key      | Atom-1          | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 20                  | 0.22     | 0.06                | 0.22       |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 20                  | 0.22     | 0.06                | 0.22       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 20                  | 0.22     | 0.06                | 0.22       |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H    | 20                  | 0.18     | 0.03                | 0.17       |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 20                  | 0.15     | 0.03                | 0.14       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 20                  | 0.12     | 0.01                | 0.12       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG11 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG11 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG12 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG12 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG13 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG13 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG21 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG21 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG22 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG22 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG23 | 20                  | 0.11     | 0.0                 | 0.11       |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG23 | 20                  | 0.11     | 0.0                 | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD22  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD13  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,3197) | 1:132:A:GLU:HB2  | 1:15:A:LEU:HD22  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD23  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD11  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD12  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD21  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,3197) | 1:132:A:GLU:HB2  | 1:15:A:LEU:HD21  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,3197) | 1:132:A:GLU:HB2  | 1:15:A:LEU:HD23  | 19                  | 1.39     | 0.48                | 1.48       |
| (1,2127) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD11 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD12 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD13 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD13 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD23 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD21 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD21 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD12 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2127) | 1:158:A:LEU:HD22 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD11 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD12 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD13 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD13 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD23 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD21 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD21 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD12 | 1:55:A:LEU:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2378) | 1:158:A:LEU:HD22 | 1:54:A:VAL:HA    | 19                  | 0.9      | 0.33                | 0.94       |
| (1,2178) | 1:26:A:MET:HE2   | 1:69:A:ASN:HB3   | 19                  | 0.84     | 0.24                | 0.94       |
| (1,2178) | 1:26:A:MET:HE1   | 1:26:A:MET:HB3   | 19                  | 0.84     | 0.24                | 0.94       |
| (1,2178) | 1:26:A:MET:HE3   | 1:26:A:MET:HB3   | 19                  | 0.84     | 0.24                | 0.94       |
| (1,2178) | 1:26:A:MET:HE1   | 1:69:A:ASN:HB3   | 19                  | 0.84     | 0.24                | 0.94       |
| (1,2178) | 1:26:A:MET:HE2   | 1:26:A:MET:HB3   | 19                  | 0.84     | 0.24                | 0.94       |
| (1,2178) | 1:26:A:MET:HE3   | 1:69:A:ASN:HB3   | 19                  | 0.84     | 0.24                | 0.94       |
| (1,2178) | 1:26:A:MET:HE2   | 1:26:A:MET:HB2   | 19                  | 0.84     | 0.24                | 0.94       |
| (1,2178) | 1:26:A:MET:HE3   | 1:26:A:MET:HB2   | 19                  | 0.84     | 0.24                | 0.94       |
| (1,2979) | 1:110:A:SER:H    | 1:80:A:ILE:HG13  | 19                  | 0.53     | 0.17                | 0.5        |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG22 | 19                  | 0.53     | 0.17                | 0.5        |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG21 | 19                  | 0.53     | 0.17                | 0.5        |
| (1,2979) | 1:110:A:SER:H    | 1:80:A:ILE:HG12  | 19                  | 0.53     | 0.17                | 0.5        |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG23 | 19                  | 0.53     | 0.17                | 0.5        |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2916) | 1:96:A:ILE:H    | 1:39:A:LYS:HG2   | 19                  | 0.49     | 0.21                | 0.55       |
| (1,2916) | 1:96:A:ILE:H    | 1:39:A:LYS:HG3   | 19                  | 0.49     | 0.21                | 0.55       |
| (1,2916) | 1:96:A:ILE:H    | 1:102:A:LEU:HB2  | 19                  | 0.49     | 0.21                | 0.55       |
| (1,2716) | 1:19:A:LEU:H    | 1:28:A:ALA:HB2   | 19                  | 0.35     | 0.12                | 0.33       |
| (1,2716) | 1:19:A:LEU:H    | 1:28:A:ALA:HB1   | 19                  | 0.35     | 0.12                | 0.33       |
| (1,2716) | 1:19:A:LEU:H    | 1:28:A:ALA:HB3   | 19                  | 0.35     | 0.12                | 0.33       |
| (1,2716) | 1:19:A:LEU:H    | 1:29:A:LEU:HB2   | 19                  | 0.35     | 0.12                | 0.33       |
| (1,2561) | 1:101:A:ILE:H   | 1:101:A:ILE:HD11 | 19                  | 0.33     | 0.04                | 0.34       |
| (1,2561) | 1:101:A:ILE:H   | 1:101:A:ILE:HD12 | 19                  | 0.33     | 0.04                | 0.34       |
| (1,2561) | 1:101:A:ILE:H   | 1:101:A:ILE:HD13 | 19                  | 0.33     | 0.04                | 0.34       |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD12  | 19                  | 0.29     | 0.01                | 0.29       |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD13  | 19                  | 0.29     | 0.01                | 0.29       |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD11  | 19                  | 0.29     | 0.01                | 0.29       |
| (1,3065) | 1:92:A:VAL:HG11 | 1:93:A:THR:H     | 19                  | 0.28     | 0.11                | 0.25       |
| (1,3065) | 1:92:A:VAL:HG12 | 1:93:A:THR:H     | 19                  | 0.28     | 0.11                | 0.25       |
| (1,3065) | 1:92:A:VAL:HG13 | 1:93:A:THR:H     | 19                  | 0.28     | 0.11                | 0.25       |
| (1,3159) | 1:15:A:LEU:HD12 | 1:131:A:ILE:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD22 | 1:131:A:ILE:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD13 | 1:136:A:GLN:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD23 | 1:131:A:ILE:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD22 | 1:136:A:GLN:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD21 | 1:136:A:GLN:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD12 | 1:136:A:GLN:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD13 | 1:131:A:ILE:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD21 | 1:131:A:ILE:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,3159) | 1:15:A:LEU:HD23 | 1:136:A:GLN:H    | 18                  | 0.81     | 0.43                | 0.78       |
| (1,2411) | 1:102:A:LEU:H   | 1:96:A:ILE:HD12  | 18                  | 0.74     | 0.24                | 0.71       |
| (1,2411) | 1:102:A:LEU:H   | 1:101:A:ILE:HD13 | 18                  | 0.74     | 0.24                | 0.71       |
| (1,2411) | 1:102:A:LEU:H   | 1:96:A:ILE:HD13  | 18                  | 0.74     | 0.24                | 0.71       |
| (1,2411) | 1:102:A:LEU:H   | 1:96:A:ILE:HD11  | 18                  | 0.74     | 0.24                | 0.71       |
| (1,2411) | 1:102:A:LEU:H   | 1:101:A:ILE:HD11 | 18                  | 0.74     | 0.24                | 0.71       |
| (1,2411) | 1:102:A:LEU:H   | 1:101:A:ILE:HD12 | 18                  | 0.74     | 0.24                | 0.71       |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD13  | 18                  | 0.68     | 0.22                | 0.74       |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD12  | 18                  | 0.68     | 0.22                | 0.74       |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD11  | 18                  | 0.68     | 0.22                | 0.74       |
| (1,2761) | 1:30:A:ILE:H    | 1:17:A:LEU:HD13  | 18                  | 0.68     | 0.22                | 0.74       |
| (1,2881) | 1:17:A:LEU:H    | 1:15:A:LEU:HB3   | 18                  | 0.62     | 0.23                | 0.59       |
| (1,2881) | 1:17:A:LEU:H    | 1:31:A:LYS:HB2   | 18                  | 0.62     | 0.23                | 0.59       |
| (1,2881) | 1:17:A:LEU:H    | 1:15:A:LEU:HB2   | 18                  | 0.62     | 0.23                | 0.59       |
| (1,2881) | 1:17:A:LEU:H    | 1:31:A:LYS:HB3   | 18                  | 0.62     | 0.23                | 0.59       |
| (1,2550) | 1:95:A:ASP:H    | 1:102:A:LEU:HB2  | 18                  | 0.61     | 0.15                | 0.56       |
| (1,2550) | 1:95:A:ASP:H    | 1:39:A:LYS:HB2   | 18                  | 0.61     | 0.15                | 0.56       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3179) | 1:35:A:THR:HB   | 1:36:A:ILE:HG12  | 18                  | 0.55     | 0.22                | 0.68       |
| (1,2404) | 1:92:A:VAL:H    | 1:41:A:THR:HG22  | 18                  | 0.38     | 0.11                | 0.36       |
| (1,2404) | 1:92:A:VAL:H    | 1:41:A:THR:HG23  | 18                  | 0.38     | 0.11                | 0.36       |
| (1,2404) | 1:92:A:VAL:H    | 1:41:A:THR:HG21  | 18                  | 0.38     | 0.11                | 0.36       |
| (1,2447) | 1:97:A:ASP:H    | 1:101:A:ILE:HD11 | 18                  | 0.37     | 0.19                | 0.38       |
| (1,2447) | 1:97:A:ASP:H    | 1:101:A:ILE:HD12 | 18                  | 0.37     | 0.19                | 0.38       |
| (1,2447) | 1:97:A:ASP:H    | 1:96:A:ILE:HD12  | 18                  | 0.37     | 0.19                | 0.38       |
| (1,2447) | 1:97:A:ASP:H    | 1:101:A:ILE:HD13 | 18                  | 0.37     | 0.19                | 0.38       |
| (1,2642) | 1:46:A:THR:H    | 1:45:A:THR:HG21  | 18                  | 0.36     | 0.13                | 0.34       |
| (1,2642) | 1:46:A:THR:H    | 1:45:A:THR:HG22  | 18                  | 0.36     | 0.13                | 0.34       |
| (1,2642) | 1:46:A:THR:H    | 1:45:A:THR:HG23  | 18                  | 0.36     | 0.13                | 0.34       |
| (1,3180) | 1:35:A:THR:HA   | 1:36:A:ILE:HG12  | 18                  | 0.27     | 0.1                 | 0.26       |
| (1,2604) | 1:43:A:ILE:H    | 1:43:A:ILE:HD13  | 17                  | 0.42     | 0.23                | 0.32       |
| (1,2604) | 1:43:A:ILE:H    | 1:43:A:ILE:HD12  | 17                  | 0.42     | 0.23                | 0.32       |
| (1,2604) | 1:43:A:ILE:H    | 1:43:A:ILE:HD11  | 17                  | 0.42     | 0.23                | 0.32       |
| (1,2604) | 1:43:A:ILE:H    | 1:43:A:ILE:HG22  | 17                  | 0.42     | 0.23                | 0.32       |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG21  | 17                  | 0.38     | 0.16                | 0.43       |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG13  | 17                  | 0.38     | 0.16                | 0.43       |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG22  | 17                  | 0.38     | 0.16                | 0.43       |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG23  | 17                  | 0.38     | 0.16                | 0.43       |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG11  | 17                  | 0.38     | 0.16                | 0.43       |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG12  | 17                  | 0.38     | 0.16                | 0.43       |
| (1,2169) | 1:56:A:ILE:HG22 | 1:74:A:ARG:HB2   | 17                  | 0.37     | 0.21                | 0.29       |
| (1,2169) | 1:56:A:ILE:HG21 | 1:58:A:VAL:HB    | 17                  | 0.37     | 0.21                | 0.29       |
| (1,2169) | 1:56:A:ILE:HG23 | 1:58:A:VAL:HB    | 17                  | 0.37     | 0.21                | 0.29       |
| (1,2169) | 1:56:A:ILE:HG22 | 1:58:A:VAL:HB    | 17                  | 0.37     | 0.21                | 0.29       |
| (1,2169) | 1:56:A:ILE:HG22 | 1:158:A:LEU:HG   | 17                  | 0.37     | 0.21                | 0.29       |
| (1,3155) | 1:14:A:PRO:HA   | 1:13:A:ALA:HB2   | 17                  | 0.23     | 0.05                | 0.23       |
| (1,3155) | 1:14:A:PRO:HA   | 1:13:A:ALA:HB1   | 17                  | 0.23     | 0.05                | 0.23       |
| (1,3155) | 1:14:A:PRO:HA   | 1:13:A:ALA:HB3   | 17                  | 0.23     | 0.05                | 0.23       |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG3  | 17                  | 0.21     | 0.05                | 0.21       |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG2  | 17                  | 0.21     | 0.05                | 0.21       |
| (1,2175) | 1:26:A:MET:HE3  | 1:58:A:VAL:HA    | 16                  | 0.55     | 0.25                | 0.55       |
| (1,2175) | 1:26:A:MET:HE3  | 1:16:A:SER:HA    | 16                  | 0.55     | 0.25                | 0.55       |
| (1,2175) | 1:26:A:MET:HE1  | 1:58:A:VAL:HA    | 16                  | 0.55     | 0.25                | 0.55       |
| (1,2175) | 1:26:A:MET:HE2  | 1:16:A:SER:HA    | 16                  | 0.55     | 0.25                | 0.55       |
| (1,2175) | 1:26:A:MET:HE1  | 1:16:A:SER:HA    | 16                  | 0.55     | 0.25                | 0.55       |
| (1,2175) | 1:26:A:MET:HE2  | 1:58:A:VAL:HA    | 16                  | 0.55     | 0.25                | 0.55       |
| (1,2109) | 1:66:A:THR:HG22 | 1:27:A:THR:H     | 16                  | 0.46     | 0.16                | 0.48       |
| (1,2109) | 1:66:A:THR:HG21 | 1:27:A:THR:H     | 16                  | 0.46     | 0.16                | 0.48       |
| (1,2109) | 1:66:A:THR:HG23 | 1:27:A:THR:H     | 16                  | 0.46     | 0.16                | 0.48       |
| (1,3045) | 1:33:A:ASN:HA   | 1:13:A:ALA:H     | 16                  | 0.46     | 0.18                | 0.44       |

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| Key      | Atom-1         | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3045) | 1:14:A:PRO:HD3 | 1:13:A:ALA:H     | 16                  | 0.46     | 0.18                | 0.44       |
| (1,3045) | 1:53:A:GLY:HA2 | 1:77:A:LEU:H     | 16                  | 0.46     | 0.18                | 0.44       |
| (1,2743) | 1:135:A:VAL:H  | 1:134:A:MET:HG2  | 15                  | 0.44     | 0.16                | 0.42       |
| (1,2743) | 1:135:A:VAL:H  | 1:134:A:MET:HG3  | 15                  | 0.44     | 0.16                | 0.42       |
| (1,2549) | 1:95:A:ASP:H   | 1:93:A:THR:HG21  | 15                  | 0.43     | 0.19                | 0.39       |
| (1,2549) | 1:95:A:ASP:H   | 1:93:A:THR:HG23  | 15                  | 0.43     | 0.19                | 0.39       |
| (1,2549) | 1:95:A:ASP:H   | 1:93:A:THR:HG22  | 15                  | 0.43     | 0.19                | 0.39       |
| (1,2549) | 1:95:A:ASP:H   | 1:102:A:LEU:HG   | 15                  | 0.43     | 0.19                | 0.39       |
| (1,2549) | 1:95:A:ASP:H   | 1:96:A:ILE:HG13  | 15                  | 0.43     | 0.19                | 0.39       |
| (1,2344) | 1:256:A:VAL:HA | 1:255:A:GLU:HG2  | 15                  | 0.24     | 0.08                | 0.25       |
| (1,2344) | 1:253:A:ILE:HA | 1:254:A:GLU:HG2  | 15                  | 0.24     | 0.08                | 0.25       |
| (1,2344) | 1:253:A:ILE:HA | 1:254:A:GLU:HG3  | 15                  | 0.24     | 0.08                | 0.25       |
| (1,2344) | 1:256:A:VAL:HA | 1:255:A:GLU:HG3  | 15                  | 0.24     | 0.08                | 0.25       |
| (1,2344) | 1:253:A:ILE:HA | 1:255:A:GLU:HG2  | 15                  | 0.24     | 0.08                | 0.25       |
| (1,2649) | 1:100:A:GLY:H  | 1:98:A:ALA:HB2   | 15                  | 0.2      | 0.08                | 0.19       |
| (1,2649) | 1:100:A:GLY:H  | 1:98:A:ALA:HB1   | 15                  | 0.2      | 0.08                | 0.19       |
| (1,2649) | 1:100:A:GLY:H  | 1:98:A:ALA:HB3   | 15                  | 0.2      | 0.08                | 0.19       |
| (1,1933) | 1:64:A:ALA:HB1 | 1:145:A:ASP:HB2  | 15                  | 0.14     | 0.04                | 0.12       |
| (1,1933) | 1:64:A:ALA:HB2 | 1:145:A:ASP:HB2  | 15                  | 0.14     | 0.04                | 0.12       |
| (1,1933) | 1:64:A:ALA:HB3 | 1:145:A:ASP:HB2  | 15                  | 0.14     | 0.04                | 0.12       |
| (1,2412) | 1:102:A:LEU:H  | 1:118:A:THR:HG22 | 14                  | 0.32     | 0.18                | 0.24       |
| (1,2412) | 1:102:A:LEU:H  | 1:118:A:THR:HG21 | 14                  | 0.32     | 0.18                | 0.24       |
| (1,2412) | 1:102:A:LEU:H  | 1:118:A:THR:HG23 | 14                  | 0.32     | 0.18                | 0.24       |
| (1,2868) | 1:12:A:VAL:H   | 1:12:A:VAL:HB    | 14                  | 0.31     | 0.08                | 0.3        |
| (1,2868) | 1:12:A:VAL:H   | 1:10:A:LEU:HB3   | 14                  | 0.31     | 0.08                | 0.3        |
| (1,2868) | 1:12:A:VAL:H   | 1:10:A:LEU:HG    | 14                  | 0.31     | 0.08                | 0.3        |
| (1,2868) | 1:12:A:VAL:H   | 1:10:A:LEU:HB2   | 14                  | 0.31     | 0.08                | 0.3        |
| (1,2274) | 1:116:A:LYS:HA | 1:116:A:LYS:HE3  | 13                  | 0.85     | 0.2                 | 0.88       |
| (1,2274) | 1:115:A:ASN:HA | 1:116:A:LYS:HE2  | 13                  | 0.85     | 0.2                 | 0.88       |
| (1,2274) | 1:116:A:LYS:HA | 1:116:A:LYS:HE2  | 13                  | 0.85     | 0.2                 | 0.88       |
| (1,2996) | 1:146:A:GLU:H  | 1:142:A:LYS:HG3  | 13                  | 0.6      | 0.21                | 0.58       |
| (1,2996) | 1:146:A:GLU:H  | 1:142:A:LYS:HG2  | 13                  | 0.6      | 0.21                | 0.58       |
| (1,2996) | 1:146:A:GLU:H  | 1:143:A:ALA:HB2  | 13                  | 0.6      | 0.21                | 0.58       |
| (1,2996) | 1:146:A:GLU:H  | 1:143:A:ALA:HB1  | 13                  | 0.6      | 0.21                | 0.58       |
| (1,2996) | 1:146:A:GLU:H  | 1:143:A:ALA:HB3  | 13                  | 0.6      | 0.21                | 0.58       |
| (1,2430) | 1:27:A:THR:H   | 1:19:A:LEU:HD12  | 13                  | 0.56     | 0.25                | 0.57       |
| (1,2430) | 1:27:A:THR:H   | 1:29:A:LEU:HD12  | 13                  | 0.56     | 0.25                | 0.57       |
| (1,2430) | 1:27:A:THR:H   | 1:29:A:LEU:HD13  | 13                  | 0.56     | 0.25                | 0.57       |
| (1,2430) | 1:27:A:THR:H   | 1:29:A:LEU:HD11  | 13                  | 0.56     | 0.25                | 0.57       |
| (1,2430) | 1:27:A:THR:H   | 1:19:A:LEU:HD13  | 13                  | 0.56     | 0.25                | 0.57       |
| (1,2949) | 1:69:A:ASN:H   | 1:68:A:ASP:HB2   | 13                  | 0.4      | 0.1                 | 0.41       |
| (1,2949) | 1:69:A:ASN:H   | 1:68:A:ASP:HB3   | 13                  | 0.4      | 0.1                 | 0.41       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1963) | 1:80:A:ILE:HD13 | 1:90:A:ILE:HA    | 13                  | 0.36     | 0.22                | 0.3        |
| (1,1963) | 1:80:A:ILE:HD12 | 1:77:A:LEU:HA    | 13                  | 0.36     | 0.22                | 0.3        |
| (1,1963) | 1:80:A:ILE:HD12 | 1:52:A:PRO:HA    | 13                  | 0.36     | 0.22                | 0.3        |
| (1,1963) | 1:80:A:ILE:HD13 | 1:77:A:LEU:HA    | 13                  | 0.36     | 0.22                | 0.3        |
| (1,1963) | 1:80:A:ILE:HD11 | 1:52:A:PRO:HA    | 13                  | 0.36     | 0.22                | 0.3        |
| (1,2358) | 1:45:A:THR:HA   | 1:90:A:ILE:HD13  | 12                  | 0.66     | 0.2                 | 0.67       |
| (1,2358) | 1:45:A:THR:HA   | 1:90:A:ILE:HD12  | 12                  | 0.66     | 0.2                 | 0.67       |
| (1,2358) | 1:45:A:THR:HA   | 1:90:A:ILE:HD11  | 12                  | 0.66     | 0.2                 | 0.67       |
| (1,2358) | 1:45:A:THR:HA   | 1:158:A:LEU:HD13 | 12                  | 0.66     | 0.2                 | 0.67       |
| (1,2582) | 1:51:A:GLN:H    | 1:48:A:SER:HB2   | 12                  | 0.29     | 0.15                | 0.24       |
| (1,2582) | 1:51:A:GLN:H    | 1:85:A:ARG:HA    | 12                  | 0.29     | 0.15                | 0.24       |
| (1,2567) | 1:113:A:LYS:H   | 1:111:A:THR:HG22 | 12                  | 0.27     | 0.09                | 0.28       |
| (1,2567) | 1:113:A:LYS:H   | 1:111:A:THR:HG21 | 12                  | 0.27     | 0.09                | 0.28       |
| (1,2567) | 1:113:A:LYS:H   | 1:114:A:ALA:HB3  | 12                  | 0.27     | 0.09                | 0.28       |
| (1,2567) | 1:113:A:LYS:H   | 1:111:A:THR:HG23 | 12                  | 0.27     | 0.09                | 0.28       |
| (1,2567) | 1:113:A:LYS:H   | 1:114:A:ALA:HB2  | 12                  | 0.27     | 0.09                | 0.28       |
| (1,3089) | 1:35:A:THR:HB   | 1:36:A:ILE:H     | 12                  | 0.26     | 0.09                | 0.24       |
| (1,2425) | 1:91:A:GLU:H    | 1:90:A:ILE:HG12  | 12                  | 0.17     | 0.03                | 0.17       |
| (1,2425) | 1:91:A:GLU:H    | 1:106:A:ALA:HB2  | 12                  | 0.17     | 0.03                | 0.17       |
| (1,2425) | 1:91:A:GLU:H    | 1:106:A:ALA:HB3  | 12                  | 0.17     | 0.03                | 0.17       |
| (1,2425) | 1:91:A:GLU:H    | 1:106:A:ALA:HB1  | 12                  | 0.17     | 0.03                | 0.17       |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2  | 12                  | 0.15     | 0.02                | 0.15       |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB3  | 12                  | 0.15     | 0.02                | 0.15       |
| (1,2689) | 1:45:A:THR:H    | 1:158:A:LEU:HD22 | 11                  | 0.98     | 0.33                | 1.18       |
| (1,2689) | 1:45:A:THR:H    | 1:158:A:LEU:HD11 | 11                  | 0.98     | 0.33                | 1.18       |
| (1,2689) | 1:45:A:THR:H    | 1:158:A:LEU:HD12 | 11                  | 0.98     | 0.33                | 1.18       |
| (1,2689) | 1:45:A:THR:H    | 1:158:A:LEU:HD23 | 11                  | 0.98     | 0.33                | 1.18       |
| (1,2689) | 1:45:A:THR:H    | 1:158:A:LEU:HD13 | 11                  | 0.98     | 0.33                | 1.18       |
| (1,2570) | 1:80:A:ILE:H    | 1:54:A:VAL:HG12  | 11                  | 0.74     | 0.23                | 0.74       |
| (1,2570) | 1:80:A:ILE:H    | 1:54:A:VAL:HG23  | 11                  | 0.74     | 0.23                | 0.74       |
| (1,2570) | 1:80:A:ILE:H    | 1:54:A:VAL:HG13  | 11                  | 0.74     | 0.23                | 0.74       |
| (1,2570) | 1:80:A:ILE:H    | 1:54:A:VAL:HG11  | 11                  | 0.74     | 0.23                | 0.74       |
| (1,2570) | 1:80:A:ILE:H    | 1:54:A:VAL:HG22  | 11                  | 0.74     | 0.23                | 0.74       |
| (1,2570) | 1:80:A:ILE:H    | 1:54:A:VAL:HG21  | 11                  | 0.74     | 0.23                | 0.74       |
| (1,2597) | 1:142:A:LYS:H   | 1:142:A:LYS:HG3  | 11                  | 0.55     | 0.09                | 0.55       |
| (1,2597) | 1:142:A:LYS:H   | 1:142:A:LYS:HG2  | 11                  | 0.55     | 0.09                | 0.55       |
| (1,2144) | 1:27:A:THR:HG22 | 1:156:A:ASN:HD22 | 11                  | 0.47     | 0.23                | 0.53       |
| (1,2144) | 1:27:A:THR:HG22 | 1:42:A:GLN:HE22  | 11                  | 0.47     | 0.23                | 0.53       |
| (1,2144) | 1:27:A:THR:HG21 | 1:42:A:GLN:HE21  | 11                  | 0.47     | 0.23                | 0.53       |
| (1,2144) | 1:27:A:THR:HG21 | 1:156:A:ASN:HD22 | 11                  | 0.47     | 0.23                | 0.53       |
| (1,2144) | 1:27:A:THR:HG23 | 1:42:A:GLN:HE22  | 11                  | 0.47     | 0.23                | 0.53       |
| (1,2144) | 1:27:A:THR:HG23 | 1:156:A:ASN:HD22 | 11                  | 0.47     | 0.23                | 0.53       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2144) | 1:27:A:THR:HG21  | 1:42:A:GLN:HE22  | 11                  | 0.47     | 0.23                | 0.53       |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD22  | 11                  | 0.46     | 0.19                | 0.44       |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD23  | 11                  | 0.46     | 0.19                | 0.44       |
| (1,2749) | 1:11:A:ASP:H     | 1:9:A:LEU:HD21   | 11                  | 0.46     | 0.19                | 0.44       |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD21  | 11                  | 0.46     | 0.19                | 0.44       |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD13  | 11                  | 0.46     | 0.19                | 0.44       |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HE2   | 11                  | 0.38     | 0.21                | 0.29       |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HE1   | 11                  | 0.38     | 0.21                | 0.29       |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HD1   | 11                  | 0.38     | 0.21                | 0.29       |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB1   | 11                  | 0.33     | 0.16                | 0.29       |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB3   | 11                  | 0.33     | 0.16                | 0.29       |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB2   | 11                  | 0.33     | 0.16                | 0.29       |
| (1,2824) | 1:146:A:GLU:H    | 1:143:A:ALA:HA   | 11                  | 0.23     | 0.1                 | 0.2        |
| (1,2824) | 1:146:A:GLU:H    | 1:142:A:LYS:HA   | 11                  | 0.23     | 0.1                 | 0.2        |
| (1,1673) | 1:116:A:LYS:HB2  | 1:116:A:LYS:H    | 11                  | 0.13     | 0.02                | 0.12       |
| (1,1673) | 1:116:A:LYS:HB3  | 1:116:A:LYS:H    | 11                  | 0.13     | 0.02                | 0.12       |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD11 | 10                  | 0.89     | 0.13                | 0.84       |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD12 | 10                  | 0.89     | 0.13                | 0.84       |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD13 | 10                  | 0.89     | 0.13                | 0.84       |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD21 | 10                  | 0.61     | 0.33                | 0.55       |
| (1,3156) | 1:70:A:ASN:H     | 1:15:A:LEU:HG    | 10                  | 0.61     | 0.33                | 0.55       |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD22 | 10                  | 0.61     | 0.33                | 0.55       |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD12 | 10                  | 0.61     | 0.33                | 0.55       |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD13 | 10                  | 0.61     | 0.33                | 0.55       |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD11 | 10                  | 0.61     | 0.33                | 0.55       |
| (1,2556) | 1:40:A:GLN:H     | 1:30:A:ILE:HG13  | 10                  | 0.51     | 0.22                | 0.46       |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG21  | 10                  | 0.51     | 0.22                | 0.46       |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG22  | 10                  | 0.51     | 0.22                | 0.46       |
| (1,2556) | 1:40:A:GLN:H     | 1:30:A:ILE:HG12  | 10                  | 0.51     | 0.22                | 0.46       |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG23  | 10                  | 0.51     | 0.22                | 0.46       |
| (1,2392) | 1:36:A:ILE:HD13  | 1:14:A:PRO:HD3   | 10                  | 0.5      | 0.37                | 0.36       |
| (1,2392) | 1:36:A:ILE:HG22  | 1:14:A:PRO:HD3   | 10                  | 0.5      | 0.37                | 0.36       |
| (1,2392) | 1:36:A:ILE:HD12  | 1:14:A:PRO:HD3   | 10                  | 0.5      | 0.37                | 0.36       |
| (1,2392) | 1:36:A:ILE:HD11  | 1:14:A:PRO:HD3   | 10                  | 0.5      | 0.37                | 0.36       |
| (1,2844) | 1:118:A:THR:H    | 1:117:A:ILE:HB   | 10                  | 0.43     | 0.15                | 0.49       |
| (1,2844) | 1:118:A:THR:H    | 1:116:A:LYS:HD2  | 10                  | 0.43     | 0.15                | 0.49       |
| (1,2381) | 1:104:A:VAL:HG13 | 1:19:A:LEU:HG    | 10                  | 0.35     | 0.14                | 0.33       |
| (1,2381) | 1:104:A:VAL:HG12 | 1:19:A:LEU:HG    | 10                  | 0.35     | 0.14                | 0.33       |
| (1,2381) | 1:104:A:VAL:HG11 | 1:19:A:LEU:HG    | 10                  | 0.35     | 0.14                | 0.33       |
| (1,2381) | 1:104:A:VAL:HG12 | 1:117:A:ILE:HB   | 10                  | 0.35     | 0.14                | 0.33       |
| (1,3157) | 1:24:A:GLY:H     | 1:159:A:GLU:HG3  | 10                  | 0.31     | 0.15                | 0.26       |
| (1,3157) | 1:24:A:GLY:H     | 1:152:A:VAL:HB   | 10                  | 0.31     | 0.15                | 0.26       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3157) | 1:24:A:GLY:H    | 1:159:A:GLU:HG2  | 10                  | 0.31     | 0.15                | 0.26       |
| (1,2420) | 1:119:A:ILE:H   | 1:101:A:ILE:HG21 | 10                  | 0.29     | 0.13                | 0.23       |
| (1,2420) | 1:119:A:ILE:H   | 1:117:A:ILE:HG22 | 10                  | 0.29     | 0.13                | 0.23       |
| (1,2420) | 1:119:A:ILE:H   | 1:101:A:ILE:HG22 | 10                  | 0.29     | 0.13                | 0.23       |
| (1,2420) | 1:119:A:ILE:H   | 1:101:A:ILE:HG23 | 10                  | 0.29     | 0.13                | 0.23       |
| (1,2256) | 1:94:A:PHE:HE2  | 1:19:A:LEU:HB3   | 10                  | 0.23     | 0.18                | 0.16       |
| (1,2256) | 1:94:A:PHE:HE2  | 1:19:A:LEU:HB2   | 10                  | 0.23     | 0.18                | 0.16       |
| (1,2256) | 1:94:A:PHE:HE1  | 1:19:A:LEU:HB2   | 10                  | 0.23     | 0.18                | 0.16       |
| (1,2256) | 1:44:A:PHE:HD1  | 1:19:A:LEU:HB2   | 10                  | 0.23     | 0.18                | 0.16       |
| (1,3175) | 1:157:A:ALA:HB2 | 1:44:A:PHE:HB3   | 9                   | 0.52     | 0.27                | 0.53       |
| (1,3175) | 1:64:A:ALA:HB3  | 1:149:A:ARG:HD3  | 9                   | 0.52     | 0.27                | 0.53       |
| (1,3175) | 1:64:A:ALA:HB2  | 1:149:A:ARG:HD3  | 9                   | 0.52     | 0.27                | 0.53       |
| (1,3175) | 1:157:A:ALA:HB1 | 1:44:A:PHE:HB3   | 9                   | 0.52     | 0.27                | 0.53       |
| (1,3175) | 1:64:A:ALA:HB1  | 1:149:A:ARG:HD2  | 9                   | 0.52     | 0.27                | 0.53       |
| (1,1967) | 1:80:A:ILE:HD11 | 1:54:A:VAL:HA    | 9                   | 0.43     | 0.28                | 0.42       |
| (1,1967) | 1:80:A:ILE:HD13 | 1:54:A:VAL:HA    | 9                   | 0.43     | 0.28                | 0.42       |
| (1,1967) | 1:80:A:ILE:HD12 | 1:54:A:VAL:HA    | 9                   | 0.43     | 0.28                | 0.42       |
| (1,2967) | 1:99:A:ASN:H    | 1:36:A:ILE:HD11  | 9                   | 0.37     | 0.19                | 0.45       |
| (1,2967) | 1:99:A:ASN:H    | 1:36:A:ILE:HD13  | 9                   | 0.37     | 0.19                | 0.45       |
| (1,2530) | 1:90:A:ILE:H    | 1:43:A:ILE:HG22  | 9                   | 0.31     | 0.12                | 0.32       |
| (1,2530) | 1:90:A:ILE:H    | 1:43:A:ILE:HG21  | 9                   | 0.31     | 0.12                | 0.32       |
| (1,2530) | 1:90:A:ILE:H    | 1:43:A:ILE:HG23  | 9                   | 0.31     | 0.12                | 0.32       |
| (1,3174) | 1:70:A:ASN:HD21 | 1:126:A:LEU:HB2  | 8                   | 0.45     | 0.23                | 0.4        |
| (1,3174) | 1:70:A:ASN:HD21 | 1:15:A:LEU:HB2   | 8                   | 0.45     | 0.23                | 0.4        |
| (1,3174) | 1:70:A:ASN:HD21 | 1:126:A:LEU:HB3  | 8                   | 0.45     | 0.23                | 0.4        |
| (1,3161) | 1:36:A:ILE:HD13 | 1:13:A:ALA:H     | 8                   | 0.42     | 0.14                | 0.4        |
| (1,3161) | 1:36:A:ILE:HD12 | 1:11:A:ASP:H     | 8                   | 0.42     | 0.14                | 0.4        |
| (1,3161) | 1:36:A:ILE:HD13 | 1:11:A:ASP:H     | 8                   | 0.42     | 0.14                | 0.4        |
| (1,3161) | 1:36:A:ILE:HD12 | 1:13:A:ALA:H     | 8                   | 0.42     | 0.14                | 0.4        |
| (1,3026) | 1:141:A:TYR:H   | 1:140:A:LYS:HD3  | 8                   | 0.41     | 0.21                | 0.52       |
| (1,3026) | 1:141:A:TYR:H   | 1:140:A:LYS:HD2  | 8                   | 0.41     | 0.21                | 0.52       |
| (1,3026) | 1:141:A:TYR:H   | 1:138:A:ALA:HB3  | 8                   | 0.41     | 0.21                | 0.52       |
| (1,3026) | 1:141:A:TYR:H   | 1:138:A:ALA:HB2  | 8                   | 0.41     | 0.21                | 0.52       |
| (1,2698) | 1:127:A:SER:H   | 1:130:A:GLU:HB2  | 8                   | 0.38     | 0.14                | 0.35       |
| (1,2698) | 1:127:A:SER:H   | 1:130:A:GLU:HG2  | 8                   | 0.38     | 0.14                | 0.35       |
| (1,2698) | 1:127:A:SER:H   | 1:131:A:ILE:HG13 | 8                   | 0.38     | 0.14                | 0.35       |
| (1,2698) | 1:127:A:SER:H   | 1:130:A:GLU:HG3  | 8                   | 0.38     | 0.14                | 0.35       |
| (1,3125) | 1:75:A:PHE:HD1  | 1:117:A:ILE:HG21 | 8                   | 0.36     | 0.14                | 0.34       |
| (1,3125) | 1:75:A:PHE:HD2  | 1:117:A:ILE:HG23 | 8                   | 0.36     | 0.14                | 0.34       |
| (1,3125) | 1:75:A:PHE:HD1  | 1:117:A:ILE:HG23 | 8                   | 0.36     | 0.14                | 0.34       |
| (1,3125) | 1:75:A:PHE:HD2  | 1:117:A:ILE:HG22 | 8                   | 0.36     | 0.14                | 0.34       |
| (1,3125) | 1:75:A:PHE:HD2  | 1:117:A:ILE:HG21 | 8                   | 0.36     | 0.14                | 0.34       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3052) | 1:29:A:LEU:HD21 | 1:42:A:GLN:H    | 8                   | 0.35     | 0.14                | 0.34       |
| (1,3052) | 1:29:A:LEU:HD11 | 1:42:A:GLN:H    | 8                   | 0.35     | 0.14                | 0.34       |
| (1,3052) | 1:29:A:LEU:HD22 | 1:42:A:GLN:H    | 8                   | 0.35     | 0.14                | 0.34       |
| (1,3052) | 1:29:A:LEU:HD13 | 1:42:A:GLN:H    | 8                   | 0.35     | 0.14                | 0.34       |
| (1,3177) | 1:26:A:MET:HE1  | 1:29:A:LEU:H    | 8                   | 0.35     | 0.21                | 0.3        |
| (1,3177) | 1:26:A:MET:HE2  | 1:29:A:LEU:H    | 8                   | 0.35     | 0.21                | 0.3        |
| (1,3177) | 1:26:A:MET:HE3  | 1:29:A:LEU:H    | 8                   | 0.35     | 0.21                | 0.3        |
| (1,3173) | 1:70:A:ASN:HD22 | 1:126:A:LEU:HB2 | 8                   | 0.32     | 0.1                 | 0.32       |
| (1,3173) | 1:70:A:ASN:HD22 | 1:15:A:LEU:HB2  | 8                   | 0.32     | 0.1                 | 0.32       |
| (1,3173) | 1:70:A:ASN:HD22 | 1:126:A:LEU:HB3 | 8                   | 0.32     | 0.1                 | 0.32       |
| (1,3173) | 1:70:A:ASN:HD22 | 1:15:A:LEU:HB3  | 8                   | 0.32     | 0.1                 | 0.32       |
| (1,2931) | 1:62:A:GLU:H    | 1:62:A:GLU:HG3  | 8                   | 0.27     | 0.1                 | 0.24       |
| (1,2931) | 1:62:A:GLU:H    | 1:62:A:GLU:HG2  | 8                   | 0.27     | 0.1                 | 0.24       |
| (1,2931) | 1:62:A:GLU:H    | 1:26:A:MET:HG3  | 8                   | 0.27     | 0.1                 | 0.24       |
| (1,2790) | 1:15:A:LEU:H    | 1:14:A:PRO:HG2  | 8                   | 0.26     | 0.06                | 0.27       |
| (1,2918) | 1:45:A:THR:H    | 1:158:A:LEU:HG  | 8                   | 0.23     | 0.05                | 0.22       |
| (1,3128) | 1:141:A:TYR:HD2 | 1:144:A:GLU:HG3 | 8                   | 0.2      | 0.07                | 0.19       |
| (1,3128) | 1:141:A:TYR:HD1 | 1:137:A:GLU:HG2 | 8                   | 0.2      | 0.07                | 0.19       |
| (1,3128) | 1:141:A:TYR:HD1 | 1:144:A:GLU:HG2 | 8                   | 0.2      | 0.07                | 0.19       |
| (1,3128) | 1:141:A:TYR:HD2 | 1:137:A:GLU:HG2 | 8                   | 0.2      | 0.07                | 0.19       |
| (1,3128) | 1:141:A:TYR:HD2 | 1:144:A:GLU:HG2 | 8                   | 0.2      | 0.07                | 0.19       |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG21 | 8                   | 0.15     | 0.04                | 0.14       |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG22 | 8                   | 0.15     | 0.04                | 0.14       |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG23 | 8                   | 0.15     | 0.04                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3  | 8                   | 0.14     | 0.02                | 0.14       |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB2  | 8                   | 0.14     | 0.03                | 0.13       |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB3  | 8                   | 0.14     | 0.03                | 0.13       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2815) | 1:134:A:MET:H   | 1:134:A:MET:HG3  | 7                   | 0.92     | 0.03                | 0.93       |
| (1,2815) | 1:134:A:MET:H   | 1:134:A:MET:HG2  | 7                   | 0.92     | 0.03                | 0.93       |
| (1,2815) | 1:134:A:MET:H   | 1:137:A:GLU:HG3  | 7                   | 0.92     | 0.03                | 0.93       |
| (1,2851) | 1:126:A:LEU:H   | 1:126:A:LEU:HD22 | 7                   | 0.46     | 0.17                | 0.46       |
| (1,2851) | 1:126:A:LEU:H   | 1:131:A:ILE:HD13 | 7                   | 0.46     | 0.17                | 0.46       |
| (1,2851) | 1:126:A:LEU:H   | 1:126:A:LEU:HD23 | 7                   | 0.46     | 0.17                | 0.46       |
| (1,2851) | 1:126:A:LEU:H   | 1:131:A:ILE:HD12 | 7                   | 0.46     | 0.17                | 0.46       |
| (1,2851) | 1:126:A:LEU:H   | 1:126:A:LEU:HD13 | 7                   | 0.46     | 0.17                | 0.46       |
| (1,2851) | 1:126:A:LEU:H   | 1:126:A:LEU:HD21 | 7                   | 0.46     | 0.17                | 0.46       |
| (1,2950) | 1:69:A:ASN:H    | 1:67:A:LYS:HG3   | 7                   | 0.4      | 0.18                | 0.43       |
| (1,2950) | 1:69:A:ASN:H    | 1:67:A:LYS:HG2   | 7                   | 0.4      | 0.18                | 0.43       |
| (1,3053) | 1:102:A:LEU:HB3 | 1:104:A:VAL:H    | 7                   | 0.39     | 0.25                | 0.3        |
| (1,3053) | 1:149:A:ARG:HB2 | 1:26:A:MET:H     | 7                   | 0.39     | 0.25                | 0.3        |
| (1,3151) | 1:13:A:ALA:HA   | 1:96:A:ILE:HG22  | 7                   | 0.35     | 0.16                | 0.38       |
| (1,3151) | 1:13:A:ALA:HA   | 1:96:A:ILE:HG21  | 7                   | 0.35     | 0.16                | 0.38       |
| (1,3151) | 1:38:A:THR:HB   | 1:96:A:ILE:HG21  | 7                   | 0.35     | 0.16                | 0.38       |
| (1,3151) | 1:13:A:ALA:HA   | 1:96:A:ILE:HG23  | 7                   | 0.35     | 0.16                | 0.38       |
| (1,3151) | 1:38:A:THR:HB   | 1:96:A:ILE:HG22  | 7                   | 0.35     | 0.16                | 0.38       |
| (1,2387) | 1:29:A:LEU:HD23 | 1:92:A:VAL:HG11  | 7                   | 0.34     | 0.16                | 0.24       |
| (1,2387) | 1:29:A:LEU:HD11 | 1:92:A:VAL:HG13  | 7                   | 0.34     | 0.16                | 0.24       |
| (1,2387) | 1:29:A:LEU:HD22 | 1:92:A:VAL:HG12  | 7                   | 0.34     | 0.16                | 0.24       |
| (1,2387) | 1:29:A:LEU:HD22 | 1:92:A:VAL:HG11  | 7                   | 0.34     | 0.16                | 0.24       |
| (1,2387) | 1:29:A:LEU:HD13 | 1:92:A:VAL:HG11  | 7                   | 0.34     | 0.16                | 0.24       |
| (1,1971) | 1:43:A:ILE:HD12 | 1:91:A:GLU:H     | 6                   | 0.87     | 0.41                | 0.85       |
| (1,1971) | 1:43:A:ILE:HD11 | 1:91:A:GLU:H     | 6                   | 0.87     | 0.41                | 0.85       |
| (1,1971) | 1:43:A:ILE:HD12 | 1:92:A:VAL:H     | 6                   | 0.87     | 0.41                | 0.85       |
| (1,2224) | 1:44:A:PHE:H    | 1:43:A:ILE:HD12  | 6                   | 0.73     | 0.26                | 0.83       |
| (1,2224) | 1:44:A:PHE:H    | 1:43:A:ILE:HD11  | 6                   | 0.73     | 0.26                | 0.83       |
| (1,2750) | 1:11:A:ASP:H    | 1:12:A:VAL:HG23  | 6                   | 0.44     | 0.2                 | 0.33       |
| (1,2750) | 1:11:A:ASP:H    | 1:12:A:VAL:HG13  | 6                   | 0.44     | 0.2                 | 0.33       |
| (1,2750) | 1:11:A:ASP:H    | 1:12:A:VAL:HG11  | 6                   | 0.44     | 0.2                 | 0.33       |
| (1,2750) | 1:11:A:ASP:H    | 1:12:A:VAL:HG22  | 6                   | 0.44     | 0.2                 | 0.33       |
| (1,2817) | 1:134:A:MET:H   | 1:131:A:ILE:HG22 | 6                   | 0.39     | 0.13                | 0.41       |
| (1,2817) | 1:134:A:MET:H   | 1:131:A:ILE:HG23 | 6                   | 0.39     | 0.13                | 0.41       |
| (1,2817) | 1:134:A:MET:H   | 1:15:A:LEU:HD22  | 6                   | 0.39     | 0.13                | 0.41       |
| (1,2278) | 1:140:A:LYS:HB2 | 1:137:A:GLU:HG2  | 6                   | 0.38     | 0.23                | 0.32       |
| (1,2278) | 1:133:A:ARG:HG3 | 1:137:A:GLU:HG2  | 6                   | 0.38     | 0.23                | 0.32       |
| (1,2278) | 1:140:A:LYS:HB3 | 1:137:A:GLU:HG2  | 6                   | 0.38     | 0.23                | 0.32       |
| (1,2717) | 1:19:A:LEU:H    | 1:19:A:LEU:HD21  | 6                   | 0.33     | 0.17                | 0.27       |
| (1,2717) | 1:19:A:LEU:H    | 1:29:A:LEU:HD13  | 6                   | 0.33     | 0.17                | 0.27       |
| (1,2717) | 1:19:A:LEU:H    | 1:29:A:LEU:HD11  | 6                   | 0.33     | 0.17                | 0.27       |
| (1,2717) | 1:19:A:LEU:H    | 1:29:A:LEU:HD12  | 6                   | 0.33     | 0.17                | 0.27       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3117) | 1:126:A:LEU:HB2 | 1:70:A:ASN:HD22 | 6                   | 0.29     | 0.09                | 0.31       |
| (1,3117) | 1:126:A:LEU:HB3 | 1:70:A:ASN:HD22 | 6                   | 0.29     | 0.09                | 0.31       |
| (1,3117) | 1:15:A:LEU:HB2  | 1:70:A:ASN:HD21 | 6                   | 0.29     | 0.09                | 0.31       |
| (1,3189) | 1:12:A:VAL:HG12 | 1:33:A:ASN:HA   | 6                   | 0.27     | 0.08                | 0.28       |
| (1,3189) | 1:12:A:VAL:HG11 | 1:33:A:ASN:HA   | 6                   | 0.27     | 0.08                | 0.28       |
| (1,3189) | 1:12:A:VAL:HG13 | 1:33:A:ASN:HA   | 6                   | 0.27     | 0.08                | 0.28       |
| (1,2946) | 1:68:A:ASP:H    | 1:69:A:ASN:HA   | 6                   | 0.26     | 0.12                | 0.23       |
| (1,3011) | 1:157:A:ALA:H   | 1:158:A:LEU:HG  | 6                   | 0.26     | 0.13                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2  | 6                   | 0.21     | 0.05                | 0.22       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3   | 6                   | 0.21     | 0.05                | 0.22       |
| (1,2809) | 1:132:A:GLU:H   | 1:131:A:ILE:HG22 | 6                   | 0.19     | 0.04                | 0.2        |
| (1,2809) | 1:132:A:GLU:H   | 1:131:A:ILE:HG21 | 6                   | 0.19     | 0.04                | 0.2        |
| (1,2809) | 1:132:A:GLU:H   | 1:131:A:ILE:HG23 | 6                   | 0.19     | 0.04                | 0.2        |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3   | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2   | 6                   | 0.19     | 0.07                | 0.16       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2250) | 1:87:A:VAL:HG21  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG21  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG21  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG21  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG21  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG21  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG21  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3  | 6                   | 0.19     | 0.07                | 0.16       |
| (1,2188) | 1:80:A:ILE:HG21  | 1:53:A:GLY:HA2  | 5                   | 0.59     | 0.31                | 0.68       |
| (1,2188) | 1:80:A:ILE:HG22  | 1:46:A:THR:HA   | 5                   | 0.59     | 0.31                | 0.68       |
| (1,2188) | 1:80:A:ILE:HG22  | 1:53:A:GLY:HA2  | 5                   | 0.59     | 0.31                | 0.68       |
| (1,2188) | 1:80:A:ILE:HG23  | 1:53:A:GLY:HA2  | 5                   | 0.59     | 0.31                | 0.68       |
| (1,2188) | 1:80:A:ILE:HG21  | 1:46:A:THR:HA   | 5                   | 0.59     | 0.31                | 0.68       |
| (1,2181) | 1:138:A:ALA:HB3  | 1:145:A:ASP:HB2 | 5                   | 0.5      | 0.19                | 0.49       |
| (1,2181) | 1:138:A:ALA:HB3  | 1:134:A:MET:HB3 | 5                   | 0.5      | 0.19                | 0.49       |
| (1,2181) | 1:138:A:ALA:HB1  | 1:134:A:MET:HB3 | 5                   | 0.5      | 0.19                | 0.49       |
| (1,2181) | 1:138:A:ALA:HB1  | 1:145:A:ASP:HB2 | 5                   | 0.5      | 0.19                | 0.49       |
| (1,2181) | 1:138:A:ALA:HB2  | 1:134:A:MET:HB3 | 5                   | 0.5      | 0.19                | 0.49       |
| (1,3118) | 1:131:A:ILE:HD12 | 1:70:A:ASN:HD21 | 5                   | 0.44     | 0.27                | 0.4        |
| (1,3118) | 1:126:A:LEU:HD11 | 1:70:A:ASN:HD22 | 5                   | 0.44     | 0.27                | 0.4        |
| (1,3118) | 1:126:A:LEU:HD12 | 1:70:A:ASN:HD21 | 5                   | 0.44     | 0.27                | 0.4        |
| (1,3118) | 1:131:A:ILE:HD12 | 1:70:A:ASN:HD22 | 5                   | 0.44     | 0.27                | 0.4        |
| (1,3160) | 1:143:A:ALA:HA   | 1:142:A:LYS:HB3 | 5                   | 0.43     | 0.06                | 0.46       |
| (1,3160) | 1:143:A:ALA:HA   | 1:142:A:LYS:HB2 | 5                   | 0.43     | 0.06                | 0.46       |
| (1,2748) | 1:11:A:ASP:H     | 1:36:A:ILE:HG12 | 5                   | 0.38     | 0.14                | 0.41       |
| (1,1966) | 1:119:A:ILE:HD12 | 1:119:A:ILE:HB  | 5                   | 0.27     | 0.01                | 0.27       |
| (1,1966) | 1:119:A:ILE:HD11 | 1:119:A:ILE:HB  | 5                   | 0.27     | 0.01                | 0.27       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1966) | 1:119:A:ILE:HD13 | 1:119:A:ILE:HB   | 5                   | 0.27     | 0.01                | 0.27       |
| (1,2501) | 1:31:A:LYS:H     | 1:28:A:ALA:HB3   | 5                   | 0.27     | 0.12                | 0.22       |
| (1,2501) | 1:31:A:LYS:H     | 1:28:A:ALA:HB2   | 5                   | 0.27     | 0.12                | 0.22       |
| (1,2501) | 1:31:A:LYS:H     | 1:13:A:ALA:HB3   | 5                   | 0.27     | 0.12                | 0.22       |
| (1,2495) | 1:57:A:GLN:H     | 1:55:A:LEU:HB3   | 5                   | 0.23     | 0.11                | 0.16       |
| (1,2495) | 1:57:A:GLN:H     | 1:74:A:ARG:HB3   | 5                   | 0.23     | 0.11                | 0.16       |
| (1,2495) | 1:57:A:GLN:H     | 1:74:A:ARG:HB2   | 5                   | 0.23     | 0.11                | 0.16       |
| (1,3017) | 1:12:A:VAL:H     | 1:14:A:PRO:HD3   | 5                   | 0.22     | 0.11                | 0.15       |
| (1,1455) | 1:51:A:GLN:HG2   | 1:51:A:GLN:H     | 5                   | 0.2      | 0.02                | 0.19       |
| (1,1455) | 1:51:A:GLN:HG3   | 1:51:A:GLN:H     | 5                   | 0.2      | 0.02                | 0.19       |
| (1,3008) | 1:148:A:GLN:H    | 1:151:A:ARG:HB2  | 5                   | 0.2      | 0.05                | 0.22       |
| (1,3008) | 1:148:A:GLN:H    | 1:149:A:ARG:HB3  | 5                   | 0.2      | 0.05                | 0.22       |
| (1,3135) | 1:83:A:ALA:H     | 1:82:A:PRO:HB2   | 5                   | 0.18     | 0.06                | 0.19       |
| (1,3135) | 1:83:A:ALA:H     | 1:82:A:PRO:HB3   | 5                   | 0.18     | 0.06                | 0.19       |
| (1,942)  | 1:37:A:PRO:HB2   | 1:38:A:THR:HG21  | 5                   | 0.17     | 0.04                | 0.19       |
| (1,942)  | 1:37:A:PRO:HB2   | 1:38:A:THR:HG22  | 5                   | 0.17     | 0.04                | 0.19       |
| (1,942)  | 1:37:A:PRO:HB2   | 1:38:A:THR:HG23  | 5                   | 0.17     | 0.04                | 0.19       |
| (1,942)  | 1:37:A:PRO:HB3   | 1:38:A:THR:HG21  | 5                   | 0.17     | 0.04                | 0.19       |
| (1,942)  | 1:37:A:PRO:HB3   | 1:38:A:THR:HG22  | 5                   | 0.17     | 0.04                | 0.19       |
| (1,942)  | 1:37:A:PRO:HB3   | 1:38:A:THR:HG23  | 5                   | 0.17     | 0.04                | 0.19       |
| (1,2820) | 1:136:A:GLN:H    | 1:135:A:VAL:HG13 | 5                   | 0.16     | 0.07                | 0.13       |
| (1,2820) | 1:136:A:GLN:H    | 1:135:A:VAL:HG12 | 5                   | 0.16     | 0.07                | 0.13       |
| (1,3136) | 1:113:A:LYS:HG2  | 1:112:A:GLY:H    | 4                   | 0.87     | 0.17                | 0.84       |
| (1,3136) | 1:113:A:LYS:HG3  | 1:112:A:GLY:H    | 4                   | 0.87     | 0.17                | 0.84       |
| (1,3136) | 1:109:A:LYS:HG2  | 1:112:A:GLY:H    | 4                   | 0.87     | 0.17                | 0.84       |
| (1,3172) | 1:56:A:ILE:HD11  | 1:77:A:LEU:HA    | 4                   | 0.81     | 0.39                | 0.97       |
| (1,3172) | 1:56:A:ILE:HD13  | 1:90:A:ILE:HA    | 4                   | 0.81     | 0.39                | 0.97       |
| (1,3172) | 1:56:A:ILE:HD11  | 1:90:A:ILE:HA    | 4                   | 0.81     | 0.39                | 0.97       |
| (1,2747) | 1:11:A:ASP:H     | 1:10:A:LEU:HB3   | 4                   | 0.67     | 0.14                | 0.68       |
| (1,2747) | 1:11:A:ASP:H     | 1:10:A:LEU:HG    | 4                   | 0.67     | 0.14                | 0.68       |
| (1,2873) | 1:103:A:ASN:HD21 | 1:101:A:ILE:HG21 | 4                   | 0.62     | 0.3                 | 0.58       |
| (1,2873) | 1:103:A:ASN:HD21 | 1:102:A:LEU:HD11 | 4                   | 0.62     | 0.3                 | 0.58       |
| (1,2873) | 1:103:A:ASN:HD21 | 1:101:A:ILE:HG23 | 4                   | 0.62     | 0.3                 | 0.58       |
| (1,3122) | 1:101:A:ILE:HG21 | 1:103:A:ASN:HD21 | 4                   | 0.62     | 0.3                 | 0.58       |
| (1,3122) | 1:102:A:LEU:HD11 | 1:103:A:ASN:HD21 | 4                   | 0.62     | 0.3                 | 0.58       |
| (1,3122) | 1:101:A:ILE:HG23 | 1:103:A:ASN:HD21 | 4                   | 0.62     | 0.3                 | 0.58       |
| (1,3042) | 1:19:A:LEU:HD11  | 1:59:A:TYR:H     | 4                   | 0.61     | 0.28                | 0.72       |
| (1,3042) | 1:19:A:LEU:HD13  | 1:59:A:TYR:H     | 4                   | 0.61     | 0.28                | 0.72       |
| (1,2074) | 1:11:A:ASP:HB3   | 1:36:A:ILE:HG12  | 4                   | 0.4      | 0.29                | 0.3        |
| (1,2909) | 1:147:A:VAL:H    | 1:146:A:GLU:HB2  | 4                   | 0.39     | 0.08                | 0.42       |
| (1,2909) | 1:147:A:VAL:H    | 1:146:A:GLU:HB3  | 4                   | 0.39     | 0.08                | 0.42       |
| (1,2516) | 1:96:A:ILE:H     | 1:39:A:LYS:HB2   | 4                   | 0.34     | 0.09                | 0.34       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2216) | 1:13:A:ALA:HB2  | 1:32:A:ARG:HB3   | 4                   | 0.34     | 0.14                | 0.37       |
| (1,2216) | 1:13:A:ALA:HB1  | 1:32:A:ARG:HB2   | 4                   | 0.34     | 0.14                | 0.37       |
| (1,2216) | 1:13:A:ALA:HB3  | 1:32:A:ARG:HB2   | 4                   | 0.34     | 0.14                | 0.37       |
| (1,2216) | 1:13:A:ALA:HB1  | 1:32:A:ARG:HB3   | 4                   | 0.34     | 0.14                | 0.37       |
| (1,2539) | 1:32:A:ARG:H    | 1:31:A:LYS:HB3   | 4                   | 0.31     | 0.13                | 0.3        |
| (1,2539) | 1:32:A:ARG:H    | 1:31:A:LYS:HB2   | 4                   | 0.31     | 0.13                | 0.3        |
| (1,2921) | 1:48:A:SER:H    | 1:85:A:ARG:HG3   | 4                   | 0.27     | 0.12                | 0.28       |
| (1,2921) | 1:48:A:SER:H    | 1:157:A:ALA:HB2  | 4                   | 0.27     | 0.12                | 0.28       |
| (1,2921) | 1:48:A:SER:H    | 1:85:A:ARG:HG2   | 4                   | 0.27     | 0.12                | 0.28       |
| (1,3073) | 1:77:A:LEU:HD11 | 1:115:A:ASN:H    | 4                   | 0.27     | 0.03                | 0.26       |
| (1,3073) | 1:77:A:LEU:HD13 | 1:115:A:ASN:H    | 4                   | 0.27     | 0.03                | 0.26       |
| (1,3073) | 1:77:A:LEU:HD12 | 1:115:A:ASN:H    | 4                   | 0.27     | 0.03                | 0.26       |
| (1,2972) | 1:104:A:VAL:H   | 1:117:A:ILE:HG12 | 4                   | 0.24     | 0.16                | 0.16       |
| (1,2972) | 1:104:A:VAL:H   | 1:118:A:THR:HG21 | 4                   | 0.24     | 0.16                | 0.16       |
| (1,3149) | 1:13:A:ALA:HB3  | 1:14:A:PRO:HD2   | 4                   | 0.24     | 0.06                | 0.22       |
| (1,3149) | 1:13:A:ALA:HB2  | 1:14:A:PRO:HD2   | 4                   | 0.24     | 0.06                | 0.22       |
| (1,2368) | 1:115:A:ASN:HA  | 1:75:A:PHE:HE1   | 4                   | 0.21     | 0.07                | 0.2        |
| (1,2368) | 1:115:A:ASN:HA  | 1:75:A:PHE:HE2   | 4                   | 0.21     | 0.07                | 0.2        |
| (1,2904) | 1:18:A:GLY:H    | 1:19:A:LEU:HD21  | 4                   | 0.2      | 0.08                | 0.17       |
| (1,2904) | 1:18:A:GLY:H    | 1:19:A:LEU:HD22  | 4                   | 0.2      | 0.08                | 0.17       |
| (1,2904) | 1:18:A:GLY:H    | 1:29:A:LEU:HD13  | 4                   | 0.2      | 0.08                | 0.17       |
| (1,2463) | 1:108:A:ASP:H   | 1:77:A:LEU:HG    | 4                   | 0.17     | 0.06                | 0.15       |
| (1,2009) | 1:9:A:LEU:HA    | 1:9:A:LEU:H      | 4                   | 0.14     | 0.01                | 0.14       |
| (1,2613) | 1:9:A:LEU:HA    | 1:9:A:LEU:H      | 4                   | 0.14     | 0.01                | 0.14       |
| (1,1106) | 1:35:A:THR:HG21 | 1:34:A:SER:HA    | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1106) | 1:35:A:THR:HG22 | 1:34:A:SER:HA    | 4                   | 0.12     | 0.02                | 0.12       |
| (1,1106) | 1:35:A:THR:HG23 | 1:34:A:SER:HA    | 4                   | 0.12     | 0.02                | 0.12       |
| (1,2332) | 1:17:A:LEU:H    | 1:13:A:ALA:HB3   | 3                   | 0.71     | 0.28                | 0.88       |
| (1,2332) | 1:17:A:LEU:H    | 1:13:A:ALA:HB2   | 3                   | 0.71     | 0.28                | 0.88       |
| (1,2332) | 1:17:A:LEU:H    | 1:13:A:ALA:HB1   | 3                   | 0.71     | 0.28                | 0.88       |
| (1,2568) | 1:113:A:LYS:H   | 1:113:A:LYS:HG2  | 3                   | 0.53     | 0.2                 | 0.61       |
| (1,2568) | 1:113:A:LYS:H   | 1:113:A:LYS:HG3  | 3                   | 0.53     | 0.2                 | 0.61       |
| (1,2862) | 1:86:A:GLY:H    | 1:85:A:ARG:HB3   | 3                   | 0.45     | 0.23                | 0.59       |
| (1,2862) | 1:86:A:GLY:H    | 1:45:A:THR:HG21  | 3                   | 0.45     | 0.23                | 0.59       |
| (1,2075) | 1:130:A:GLU:H   | 1:130:A:GLU:HG2  | 3                   | 0.43     | 0.18                | 0.34       |
| (1,2075) | 1:130:A:GLU:H   | 1:130:A:GLU:HG3  | 3                   | 0.43     | 0.18                | 0.34       |
| (1,2075) | 1:130:A:GLU:H   | 1:129:A:GLU:HG3  | 3                   | 0.43     | 0.18                | 0.34       |
| (1,2884) | 1:133:A:ARG:H   | 1:133:A:ARG:HG3  | 3                   | 0.43     | 0.11                | 0.5        |
| (1,2884) | 1:133:A:ARG:H   | 1:133:A:ARG:HG2  | 3                   | 0.43     | 0.11                | 0.5        |
| (1,2020) | 1:72:A:LEU:HA   | 1:72:A:LEU:HD12  | 3                   | 0.42     | 0.17                | 0.45       |
| (1,2020) | 1:72:A:LEU:HA   | 1:72:A:LEU:HD13  | 3                   | 0.42     | 0.17                | 0.45       |
| (1,2548) | 1:95:A:ASP:H    | 1:30:A:ILE:HD11  | 3                   | 0.34     | 0.01                | 0.35       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2548) | 1:95:A:ASP:H     | 1:30:A:ILE:HD12 | 3                   | 0.34     | 0.01                | 0.35       |
| (1,2548) | 1:95:A:ASP:H     | 1:30:A:ILE:HD13 | 3                   | 0.34     | 0.01                | 0.35       |
| (1,2379) | 1:158:A:LEU:HD11 | 1:44:A:PHE:H    | 3                   | 0.32     | 0.13                | 0.36       |
| (1,2379) | 1:158:A:LEU:HD23 | 1:21:A:THR:H    | 3                   | 0.32     | 0.13                | 0.36       |
| (1,2842) | 1:140:A:LYS:H    | 1:139:A:GLU:HB2 | 3                   | 0.3      | 0.14                | 0.23       |
| (1,2980) | 1:111:A:THR:H    | 1:81:A:PRO:HG3  | 3                   | 0.27     | 0.09                | 0.33       |
| (1,2526) | 1:42:A:GLN:H     | 1:94:A:PHE:H    | 3                   | 0.23     | 0.04                | 0.24       |
| (1,2182) | 1:54:A:VAL:HG23  | 1:76:A:GLU:HA   | 3                   | 0.22     | 0.06                | 0.22       |
| (1,2182) | 1:54:A:VAL:HG23  | 1:77:A:LEU:HA   | 3                   | 0.22     | 0.06                | 0.22       |
| (1,2503) | 1:31:A:LYS:H     | 1:30:A:ILE:HG12 | 3                   | 0.21     | 0.02                | 0.22       |
| (1,2999) | 1:140:A:LYS:H    | 1:141:A:TYR:HB2 | 3                   | 0.18     | 0.05                | 0.19       |
| (1,2429) | 1:27:A:THR:H     | 1:25:A:VAL:HB   | 3                   | 0.17     | 0.04                | 0.19       |
| (1,2429) | 1:27:A:THR:H     | 1:26:A:MET:HE1  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,2429) | 1:27:A:THR:H     | 1:26:A:MET:HE3  | 3                   | 0.17     | 0.04                | 0.19       |
| (1,2944) | 1:68:A:ASP:H     | 1:68:A:ASP:HB2  | 3                   | 0.17     | 0.03                | 0.17       |
| (1,94)   | 1:253:A:ILE:HB   | 1:253:A:ILE:HA  | 3                   | 0.16     | 0.01                | 0.16       |
| (1,1752) | 1:22:A:ALA:HB1   | 1:47:A:TYR:H    | 3                   | 0.13     | 0.03                | 0.11       |
| (1,1752) | 1:22:A:ALA:HB2   | 1:47:A:TYR:H    | 3                   | 0.13     | 0.03                | 0.11       |
| (1,1752) | 1:22:A:ALA:HB3   | 1:47:A:TYR:H    | 3                   | 0.13     | 0.03                | 0.11       |
| (1,2219) | 1:204:A:GLU:HA   | 1:203:A:ALA:H   | 3                   | 0.13     | 0.01                | 0.13       |
| (1,2696) | 1:127:A:SER:H    | 1:127:A:SER:HA  | 3                   | 0.13     | 0.01                | 0.12       |
| (1,1621) | 1:67:A:LYS:HG2   | 1:68:A:ASP:H    | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1621) | 1:67:A:LYS:HG3   | 1:68:A:ASP:H    | 3                   | 0.12     | 0.02                | 0.11       |
| (1,937)  | 1:39:A:LYS:HA    | 1:38:A:THR:HG21 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,937)  | 1:39:A:LYS:HA    | 1:38:A:THR:HG22 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,937)  | 1:39:A:LYS:HA    | 1:38:A:THR:HG23 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD11 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD11 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD12 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD12 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD13 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD13 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD21 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD21 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD22 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD22 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD23 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB2   | 1:17:A:LEU:HD23 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD11 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD11 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD12 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD12 | 3                   | 0.12     | 0.02                | 0.11       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD13 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD13 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD21 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD21 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD22 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD22 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD23 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,2062) | 1:17:A:LEU:HB3   | 1:17:A:LEU:HD23 | 3                   | 0.12     | 0.02                | 0.11       |
| (1,1187) | 1:62:A:GLU:HB2   | 1:60:A:GLU:HA   | 3                   | 0.12     | 0.01                | 0.11       |
| (1,1187) | 1:62:A:GLU:HB3   | 1:60:A:GLU:HA   | 3                   | 0.12     | 0.01                | 0.11       |
| (1,3115) | 1:131:A:ILE:HG12 | 1:70:A:ASN:HD21 | 2                   | 1.01     | 0.08                | 1.01       |
| (1,2826) | 1:146:A:GLU:H    | 1:146:A:GLU:HG3 | 2                   | 0.86     | 0.06                | 0.86       |
| (1,2154) | 1:104:A:VAL:HG12 | 1:75:A:PHE:HE1  | 2                   | 0.62     | 0.44                | 0.62       |
| (1,2154) | 1:104:A:VAL:HG12 | 1:75:A:PHE:HE2  | 2                   | 0.62     | 0.44                | 0.62       |
| (1,2324) | 1:139:A:GLU:HG2  | 1:142:A:LYS:HG2 | 2                   | 0.53     | 0.03                | 0.53       |
| (1,2593) | 1:64:A:ALA:H     | 1:66:A:THR:HA   | 2                   | 0.52     | 0.16                | 0.52       |
| (1,2593) | 1:64:A:ALA:H     | 1:63:A:ARG:HD2  | 2                   | 0.52     | 0.16                | 0.52       |
| (1,2896) | 1:16:A:SER:H     | 1:32:A:ARG:HB3  | 2                   | 0.5      | 0.08                | 0.5        |
| (1,3056) | 1:74:A:ARG:HB3   | 1:58:A:VAL:H    | 2                   | 0.49     | 0.26                | 0.49       |
| (1,2200) | 1:96:A:ILE:HD12  | 1:38:A:THR:H    | 2                   | 0.48     | 0.07                | 0.48       |
| (1,2200) | 1:96:A:ILE:HD13  | 1:38:A:THR:H    | 2                   | 0.48     | 0.07                | 0.48       |
| (1,2222) | 1:158:A:LEU:HD21 | 1:56:A:ILE:HG22 | 2                   | 0.48     | 0.13                | 0.48       |
| (1,2222) | 1:158:A:LEU:HD21 | 1:19:A:LEU:HD11 | 2                   | 0.48     | 0.13                | 0.48       |
| (1,2199) | 1:117:A:ILE:HD13 | 1:75:A:PHE:H    | 2                   | 0.47     | 0.13                | 0.47       |
| (1,2199) | 1:117:A:ILE:HD11 | 1:75:A:PHE:H    | 2                   | 0.47     | 0.13                | 0.47       |
| (1,3069) | 1:75:A:PHE:HD2   | 1:75:A:PHE:H    | 2                   | 0.46     | 0.01                | 0.46       |
| (1,3069) | 1:75:A:PHE:HE1   | 1:115:A:ASN:H   | 2                   | 0.46     | 0.01                | 0.46       |
| (1,3092) | 1:30:A:ILE:HG13  | 1:30:A:ILE:H    | 2                   | 0.46     | 0.04                | 0.46       |
| (1,2039) | 1:74:A:ARG:HA    | 1:55:A:LEU:HD12 | 2                   | 0.44     | 0.08                | 0.44       |
| (1,2039) | 1:74:A:ARG:HA    | 1:55:A:LEU:HD13 | 2                   | 0.44     | 0.08                | 0.44       |
| (1,2220) | 1:143:A:ALA:HB2  | 1:146:A:GLU:HB2 | 2                   | 0.4      | 0.12                | 0.4        |
| (1,2220) | 1:143:A:ALA:HB1  | 1:146:A:GLU:HB2 | 2                   | 0.4      | 0.12                | 0.4        |
| (1,2544) | 1:114:A:ALA:H    | 1:113:A:LYS:HB2 | 2                   | 0.4      | 0.11                | 0.4        |
| (1,2544) | 1:114:A:ALA:H    | 1:113:A:LYS:HB3 | 2                   | 0.4      | 0.11                | 0.4        |
| (1,2675) | 1:76:A:GLU:H     | 1:55:A:LEU:HD12 | 2                   | 0.38     | 0.24                | 0.38       |
| (1,2675) | 1:76:A:GLU:H     | 1:55:A:LEU:HD23 | 2                   | 0.38     | 0.24                | 0.38       |
| (1,2228) | 1:88:A:PRO:HG2   | 1:88:A:PRO:HA   | 2                   | 0.34     | 0.01                | 0.34       |
| (1,3006) | 1:145:A:ASP:H    | 1:144:A:GLU:HB2 | 2                   | 0.31     | 0.01                | 0.31       |
| (1,2776) | 1:20:A:GLU:H     | 1:56:A:ILE:HG21 | 2                   | 0.3      | 0.14                | 0.3        |
| (1,2776) | 1:20:A:GLU:H     | 1:66:A:THR:HG21 | 2                   | 0.3      | 0.14                | 0.3        |
| (1,2122) | 1:29:A:LEU:HD21  | 1:93:A:THR:HA   | 2                   | 0.3      | 0.05                | 0.3        |
| (1,2527) | 1:104:A:VAL:H    | 1:75:A:PHE:HE1  | 2                   | 0.25     | 0.07                | 0.25       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2960) | 1:86:A:GLY:H    | 1:87:A:VAL:HG21  | 2                   | 0.24     | 0.04                | 0.24       |
| (1,2960) | 1:86:A:GLY:H    | 1:87:A:VAL:HG22  | 2                   | 0.24     | 0.04                | 0.24       |
| (1,2969) | 1:100:A:GLY:H   | 1:101:A:ILE:HD12 | 2                   | 0.24     | 0.07                | 0.24       |
| (1,2969) | 1:100:A:GLY:H   | 1:101:A:ILE:HD11 | 2                   | 0.24     | 0.07                | 0.24       |
| (1,2712) | 1:137:A:GLU:H   | 1:138:A:ALA:HB3  | 2                   | 0.22     | 0.05                | 0.22       |
| (1,2712) | 1:137:A:GLU:H   | 1:138:A:ALA:HB1  | 2                   | 0.22     | 0.05                | 0.22       |
| (1,3165) | 1:96:A:ILE:HG22 | 1:38:A:THR:H     | 2                   | 0.22     | 0.06                | 0.22       |
| (1,2940) | 1:67:A:LYS:H    | 1:68:A:ASP:HB2   | 2                   | 0.21     | 0.05                | 0.21       |
| (1,2502) | 1:31:A:LYS:H    | 1:30:A:ILE:HG12  | 2                   | 0.2      | 0.02                | 0.2        |
| (1,1982) | 1:252:A:THR:HA  | 1:253:A:ILE:HG12 | 2                   | 0.19     | 0.05                | 0.19       |
| (1,1982) | 1:252:A:THR:HA  | 1:252:A:THR:HG21 | 2                   | 0.19     | 0.05                | 0.19       |
| (1,2524) | 1:42:A:GLN:H    | 1:44:A:PHE:HD1   | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2524) | 1:42:A:GLN:H    | 1:44:A:PHE:HD2   | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2913) | 1:38:A:THR:H    | 1:37:A:PRO:HG3   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2947) | 1:69:A:ASN:H    | 1:69:A:ASN:HD22  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,2947) | 1:69:A:ASN:H    | 1:69:A:ASN:HD21  | 2                   | 0.16     | 0.05                | 0.16       |
| (1,504)  | 1:39:A:LYS:HB2  | 1:39:A:LYS:HE2   | 2                   | 0.15     | 0.05                | 0.15       |
| (1,504)  | 1:39:A:LYS:HB2  | 1:39:A:LYS:HE3   | 2                   | 0.15     | 0.05                | 0.15       |
| (1,504)  | 1:39:A:LYS:HB3  | 1:39:A:LYS:HE2   | 2                   | 0.15     | 0.05                | 0.15       |
| (1,504)  | 1:39:A:LYS:HB3  | 1:39:A:LYS:HE3   | 2                   | 0.15     | 0.05                | 0.15       |
| (1,405)  | 1:39:A:LYS:HD2  | 1:95:A:ASP:HA    | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,405)  | 1:39:A:LYS:HD3  | 1:95:A:ASP:HA    | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,1785) | 1:67:A:LYS:HA   | 1:69:A:ASN:H     | 2                   | 0.14     | 0.03                | 0.14       |
| (1,2805) | 1:132:A:GLU:H   | 1:129:A:GLU:HA   | 2                   | 0.14     | 0.04                | 0.14       |
| (1,3086) | 1:26:A:MET:HE2  | 1:19:A:LEU:H     | 2                   | 0.14     | 0.02                | 0.14       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21  | 2                   | 0.13     | 0.01                | 0.13       |

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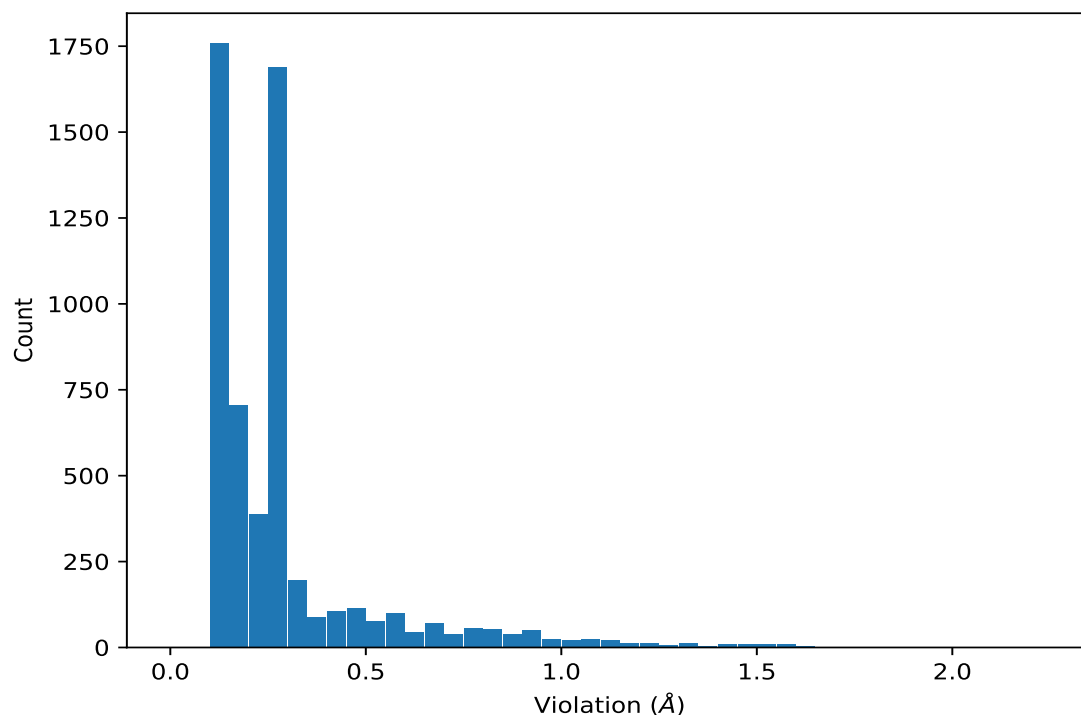
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 2                   | 0.13     | 0.01                | 0.13       |
| (1,2924) | 1:54:A:VAL:H    | 1:77:A:LEU:HD22 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,2830) | 1:138:A:ALA:H   | 1:137:A:GLU:HB2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,2831) | 1:138:A:ALA:H   | 1:137:A:GLU:HB2 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,760)  | 1:65:A:MET:HA   | 1:66:A:THR:HG21 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,760)  | 1:65:A:MET:HA   | 1:66:A:THR:HG22 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,760)  | 1:65:A:MET:HA   | 1:66:A:THR:HG23 | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,190)  | 1:142:A:LYS:HG2 | 1:139:A:GLU:HA  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,190)  | 1:142:A:LYS:HG3 | 1:139:A:GLU:HA  | 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) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3197) | 1:132:A:GLU:HB3 | 1:15:A:LEU:HD22 | 1        | 2.23          |
| (1,3197) | 1:132:A:GLU:HB3 | 1:15:A:LEU:HD13 | 2        | 1.98          |
| (1,3197) | 1:132:A:GLU:HB2 | 1:15:A:LEU:HD21 | 16       | 1.95          |
| (1,3197) | 1:132:A:GLU:HB2 | 1:15:A:LEU:HD23 | 17       | 1.75          |
| (1,3197) | 1:132:A:GLU:HB3 | 1:15:A:LEU:HD12 | 20       | 1.7           |
| (1,2159) | 1:36:A:ILE:HG23 | 1:37:A:PRO:HD3  | 3        | 1.62          |
| (1,2356) | 1:32:A:ARG:HA   | 1:15:A:LEU:HD23 | 11       | 1.61          |
| (1,2159) | 1:36:A:ILE:HG22 | 1:37:A:PRO:HD3  | 11       | 1.6           |
| (1,2159) | 1:36:A:ILE:HG22 | 1:37:A:PRO:HD3  | 14       | 1.6           |
| (1,3197) | 1:132:A:GLU:HB2 | 1:15:A:LEU:HD22 | 3        | 1.58          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3197) | 1:132:A:GLU:HB2  | 1:15:A:LEU:HD22  | 18       | 1.57          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD22  | 13       | 1.56          |
| (1,3154) | 1:46:A:THR:H     | 1:87:A:VAL:HG21  | 11       | 1.56          |
| (1,2378) | 1:158:A:LEU:HD13 | 1:55:A:LEU:HA    | 18       | 1.56          |
| (1,2127) | 1:158:A:LEU:HD13 | 1:55:A:LEU:HA    | 18       | 1.56          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD23  | 5        | 1.55          |
| (1,2159) | 1:36:A:ILE:HG23  | 1:37:A:PRO:HD3   | 9        | 1.55          |
| (1,2159) | 1:36:A:ILE:HG23  | 1:37:A:PRO:HD3   | 20       | 1.55          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG23  | 4        | 1.54          |
| (1,2159) | 1:36:A:ILE:HG23  | 1:37:A:PRO:HD3   | 4        | 1.54          |
| (1,2159) | 1:36:A:ILE:HG21  | 1:37:A:PRO:HD3   | 16       | 1.54          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 12       | 1.53          |
| (1,2159) | 1:36:A:ILE:HG23  | 1:37:A:PRO:HD3   | 1        | 1.53          |
| (1,2159) | 1:36:A:ILE:HG21  | 1:37:A:PRO:HD3   | 2        | 1.52          |
| (1,2159) | 1:36:A:ILE:HG21  | 1:37:A:PRO:HD3   | 6        | 1.52          |
| (1,2159) | 1:36:A:ILE:HG22  | 1:37:A:PRO:HD3   | 17       | 1.52          |
| (1,2159) | 1:36:A:ILE:HG23  | 1:37:A:PRO:HD3   | 5        | 1.51          |
| (1,2159) | 1:36:A:ILE:HG21  | 1:37:A:PRO:HD3   | 13       | 1.51          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD12  | 10       | 1.48          |
| (1,3159) | 1:15:A:LEU:HD12  | 1:131:A:ILE:H    | 1        | 1.48          |
| (1,3159) | 1:15:A:LEU:HD13  | 1:136:A:GLN:H    | 7        | 1.48          |
| (1,2159) | 1:36:A:ILE:HG21  | 1:37:A:PRO:HD3   | 12       | 1.47          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD13  | 6        | 1.46          |
| (1,3159) | 1:15:A:LEU:HD12  | 1:131:A:ILE:H    | 14       | 1.46          |
| (1,2481) | 1:103:A:ASN:H    | 1:30:A:ILE:HD11  | 6        | 1.46          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD13  | 11       | 1.46          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD12  | 2        | 1.46          |
| (1,2159) | 1:36:A:ILE:HG21  | 1:37:A:PRO:HD3   | 8        | 1.46          |
| (1,2159) | 1:36:A:ILE:HG22  | 1:37:A:PRO:HD3   | 10       | 1.46          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD23  | 4        | 1.45          |
| (1,2481) | 1:103:A:ASN:H    | 1:30:A:ILE:HD12  | 9        | 1.45          |
| (1,2159) | 1:36:A:ILE:HG22  | 1:37:A:PRO:HD3   | 15       | 1.45          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD11  | 17       | 1.43          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD13  | 7        | 1.42          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG21  | 10       | 1.41          |
| (1,3154) | 1:46:A:THR:H     | 1:87:A:VAL:HG23  | 20       | 1.41          |
| (1,2378) | 1:158:A:LEU:HD21 | 1:55:A:LEU:HA    | 20       | 1.41          |
| (1,2127) | 1:158:A:LEU:HD21 | 1:55:A:LEU:HA    | 20       | 1.41          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD22 | 15       | 1.37          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD21  | 1        | 1.37          |
| (1,2159) | 1:36:A:ILE:HG22  | 1:32:A:ARG:HA    | 18       | 1.37          |
| (1,1971) | 1:43:A:ILE:HD12  | 1:91:A:GLU:H     | 1        | 1.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD11  | 9        | 1.33          |
| (1,2481) | 1:103:A:ASN:H    | 1:30:A:ILE:HD13  | 2        | 1.33          |
| (1,2159) | 1:36:A:ILE:HG23  | 1:37:A:PRO:HD3   | 19       | 1.33          |
| (1,2684) | 1:158:A:LEU:H    | 1:45:A:THR:HG23  | 18       | 1.32          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD12  | 15       | 1.32          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD11  | 20       | 1.32          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD12  | 8        | 1.32          |
| (1,1971) | 1:43:A:ILE:HD11  | 1:91:A:GLU:H     | 17       | 1.32          |
| (1,2378) | 1:158:A:LEU:HD12 | 1:55:A:LEU:HA    | 12       | 1.31          |
| (1,2127) | 1:158:A:LEU:HD12 | 1:55:A:LEU:HA    | 12       | 1.31          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 3        | 1.3           |
| (1,2481) | 1:103:A:ASN:H    | 1:30:A:ILE:HD11  | 5        | 1.3           |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD21  | 4        | 1.3           |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG23  | 6        | 1.28          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD21  | 17       | 1.28          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 18       | 1.27          |
| (1,2430) | 1:27:A:THR:H     | 1:19:A:LEU:HD12  | 2        | 1.27          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 7        | 1.26          |
| (1,3193) | 1:35:A:THR:H     | 1:12:A:VAL:HG21  | 16       | 1.26          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG23  | 16       | 1.26          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 6        | 1.25          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 5        | 1.24          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 19       | 1.24          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD23 | 12       | 1.24          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD13  | 19       | 1.24          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 13       | 1.23          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD12 | 4        | 1.23          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 2        | 1.22          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD13  | 14       | 1.22          |
| (1,2159) | 1:36:A:ILE:HG23  | 1:37:A:PRO:HD3   | 7        | 1.22          |
| (1,3193) | 1:35:A:THR:H     | 1:12:A:VAL:HG22  | 20       | 1.21          |
| (1,3159) | 1:15:A:LEU:HD23  | 1:131:A:ILE:H    | 8        | 1.21          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD12 | 3        | 1.21          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD22 | 13       | 1.21          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 14       | 1.2           |
| (1,2378) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 1        | 1.2           |
| (1,2127) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 1        | 1.2           |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 10       | 1.19          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD23 | 5        | 1.18          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD13  | 18       | 1.18          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD11  | 19       | 1.18          |
| (1,3193) | 1:35:A:THR:H     | 1:12:A:VAL:HG21  | 11       | 1.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3159) | 1:15:A:LEU:HD22  | 1:131:A:ILE:H    | 6        | 1.17          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG12  | 17       | 1.17          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD22  | 12       | 1.16          |
| (1,3193) | 1:35:A:THR:H     | 1:12:A:VAL:HG21  | 4        | 1.16          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG21  | 1        | 1.16          |
| (1,3154) | 1:46:A:THR:H     | 1:87:A:VAL:HG23  | 3        | 1.16          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 12       | 1.15          |
| (1,3172) | 1:56:A:ILE:HD13  | 1:90:A:ILE:HA    | 9        | 1.14          |
| (1,3028) | 1:59:A:TYR:H     | 1:26:A:MET:HB2   | 20       | 1.14          |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD11 | 2        | 1.14          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD13  | 4        | 1.14          |
| (1,2392) | 1:36:A:ILE:HD12  | 1:14:A:PRO:HD3   | 18       | 1.14          |
| (1,3193) | 1:35:A:THR:H     | 1:12:A:VAL:HG23  | 14       | 1.13          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD11  | 20       | 1.13          |
| (1,2178) | 1:26:A:MET:HE1   | 1:26:A:MET:HB3   | 8        | 1.13          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD12  | 15       | 1.12          |
| (1,3136) | 1:113:A:LYS:HG2  | 1:112:A:GLY:H    | 1        | 1.12          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 11       | 1.12          |
| (1,2378) | 1:158:A:LEU:HD12 | 1:55:A:LEU:HA    | 15       | 1.12          |
| (1,2127) | 1:158:A:LEU:HD12 | 1:55:A:LEU:HA    | 15       | 1.12          |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD12 | 10       | 1.11          |
| (1,3141) | 1:13:A:ALA:HB1   | 1:12:A:VAL:HB    | 8        | 1.11          |
| (1,2378) | 1:158:A:LEU:HD13 | 1:54:A:VAL:HA    | 8        | 1.11          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD11  | 7        | 1.11          |
| (1,2127) | 1:158:A:LEU:HD13 | 1:54:A:VAL:HA    | 8        | 1.11          |
| (1,3193) | 1:35:A:THR:H     | 1:12:A:VAL:HG21  | 9        | 1.1           |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD22 | 5        | 1.1           |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG21  | 7        | 1.1           |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD11 | 14       | 1.1           |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD23  | 19       | 1.09          |
| (1,3193) | 1:35:A:THR:H     | 1:12:A:VAL:HG22  | 1        | 1.09          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 13       | 1.09          |
| (1,3115) | 1:131:A:ILE:HG12 | 1:70:A:ASN:HD21  | 6        | 1.09          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 12       | 1.09          |
| (1,2378) | 1:158:A:LEU:HD13 | 1:55:A:LEU:HA    | 6        | 1.09          |
| (1,2274) | 1:115:A:ASN:HA   | 1:116:A:LYS:HE2  | 13       | 1.09          |
| (1,2127) | 1:158:A:LEU:HD13 | 1:55:A:LEU:HA    | 6        | 1.09          |
| (1,3172) | 1:56:A:ILE:HD11  | 1:90:A:ILE:HA    | 11       | 1.08          |
| (1,3028) | 1:59:A:TYR:H     | 1:60:A:GLU:HG2   | 9        | 1.08          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 18       | 1.07          |
| (1,3122) | 1:102:A:LEU:HD11 | 1:103:A:ASN:HD21 | 19       | 1.07          |
| (1,2873) | 1:103:A:ASN:HD21 | 1:102:A:LEU:HD11 | 19       | 1.07          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2481) | 1:103:A:ASN:H    | 1:30:A:ILE:HD13  | 14       | 1.07          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD12  | 18       | 1.07          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 15       | 1.06          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 13       | 1.06          |
| (1,2178) | 1:26:A:MET:HE1   | 1:26:A:MET:HB3   | 2        | 1.06          |
| (1,2178) | 1:26:A:MET:HE3   | 1:26:A:MET:HB2   | 17       | 1.06          |
| (1,2178) | 1:26:A:MET:HE1   | 1:69:A:ASN:HB3   | 18       | 1.06          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 17       | 1.05          |
| (1,3150) | 1:96:A:ILE:HB    | 1:102:A:LEU:HD12 | 18       | 1.05          |
| (1,2392) | 1:36:A:ILE:HD11  | 1:14:A:PRO:HD3   | 11       | 1.05          |
| (1,2154) | 1:104:A:VAL:HG12 | 1:75:A:PHE:HE1   | 17       | 1.05          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD13  | 13       | 1.04          |
| (1,3159) | 1:15:A:LEU:HD22  | 1:131:A:ILE:H    | 2        | 1.03          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 14       | 1.03          |
| (1,2411) | 1:102:A:LEU:H    | 1:101:A:ILE:HD13 | 9        | 1.03          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD12  | 17       | 1.03          |
| (1,2411) | 1:102:A:LEU:H    | 1:101:A:ILE:HD13 | 20       | 1.03          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 6        | 1.02          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD12  | 3        | 1.02          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD11  | 12       | 1.02          |
| (1,2274) | 1:115:A:ASN:HA   | 1:116:A:LYS:HE2  | 6        | 1.02          |
| (1,2178) | 1:26:A:MET:HE2   | 1:26:A:MET:HB2   | 14       | 1.02          |
| (1,2178) | 1:26:A:MET:HE3   | 1:26:A:MET:HB3   | 20       | 1.02          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 20       | 1.01          |
| (1,2411) | 1:102:A:LEU:H    | 1:101:A:ILE:HD12 | 8        | 1.01          |
| (1,2274) | 1:116:A:LYS:HA   | 1:116:A:LYS:HE3  | 14       | 1.01          |
| (1,2178) | 1:26:A:MET:HE2   | 1:26:A:MET:HB3   | 6        | 1.01          |
| (1,2178) | 1:26:A:MET:HE3   | 1:26:A:MET:HB2   | 19       | 1.01          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD11  | 1        | 1.0           |
| (1,2411) | 1:102:A:LEU:H    | 1:101:A:ILE:HD11 | 5        | 1.0           |
| (1,2378) | 1:158:A:LEU:HD22 | 1:54:A:VAL:HA    | 14       | 1.0           |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD23  | 9        | 1.0           |
| (1,2274) | 1:116:A:LYS:HA   | 1:116:A:LYS:HE3  | 16       | 1.0           |
| (1,2127) | 1:158:A:LEU:HD22 | 1:54:A:VAL:HA    | 14       | 1.0           |
| (1,3079) | 1:105:A:THR:HG21 | 1:105:A:THR:H    | 6        | 0.99          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG22 | 2        | 0.99          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG13  | 6        | 0.99          |
| (1,2274) | 1:116:A:LYS:HA   | 1:116:A:LYS:HE3  | 4        | 0.99          |
| (1,3163) | 1:53:A:GLY:H     | 1:77:A:LEU:HB3   | 9        | 0.98          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD12  | 12       | 0.98          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 18       | 0.98          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG11  | 12       | 0.98          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2411) | 1:102:A:LEU:H    | 1:101:A:ILE:HD13 | 2        | 0.98          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD12  | 4        | 0.98          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD13  | 3        | 0.98          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD11  | 10       | 0.98          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 5        | 0.97          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG21 | 4        | 0.97          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 9        | 0.97          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG22  | 18       | 0.97          |
| (1,2224) | 1:44:A:PHE:H     | 1:43:A:ILE:HD12  | 13       | 0.97          |
| (1,2188) | 1:80:A:ILE:HG22  | 1:46:A:THR:HA    | 8        | 0.97          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 15       | 0.96          |
| (1,3079) | 1:41:A:THR:HG23  | 1:41:A:THR:H     | 10       | 0.96          |
| (1,3079) | 1:105:A:THR:HG21 | 1:105:A:THR:H    | 17       | 0.96          |
| (1,2749) | 1:11:A:ASP:H     | 1:9:A:LEU:HD21   | 11       | 0.96          |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD13 | 20       | 0.96          |
| (1,2447) | 1:97:A:ASP:H     | 1:96:A:ILE:HD12  | 12       | 0.96          |
| (1,2178) | 1:26:A:MET:HE1   | 1:26:A:MET:HB3   | 15       | 0.96          |
| (1,1956) | 1:96:A:ILE:HD12  | 1:97:A:ASP:H     | 12       | 0.96          |
| (1,3156) | 1:70:A:ASN:H     | 1:15:A:LEU:HG    | 11       | 0.95          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG23  | 2        | 0.95          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG23 | 18       | 0.95          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG13  | 4        | 0.95          |
| (1,2378) | 1:158:A:LEU:HD13 | 1:55:A:LEU:HA    | 13       | 0.95          |
| (1,2127) | 1:158:A:LEU:HD13 | 1:55:A:LEU:HA    | 13       | 0.95          |
| (1,3159) | 1:15:A:LEU:HD13  | 1:131:A:ILE:H    | 12       | 0.94          |
| (1,3159) | 1:15:A:LEU:HD23  | 1:131:A:ILE:H    | 19       | 0.94          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG22 | 5        | 0.94          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 19       | 0.94          |
| (1,2996) | 1:146:A:GLU:H    | 1:143:A:ALA:HB1  | 18       | 0.94          |
| (1,2815) | 1:134:A:MET:H    | 1:134:A:MET:HG3  | 3        | 0.94          |
| (1,2815) | 1:134:A:MET:H    | 1:134:A:MET:HG2  | 4        | 0.94          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD22 | 19       | 0.94          |
| (1,2556) | 1:40:A:GLN:H     | 1:30:A:ILE:HG13  | 1        | 0.94          |
| (1,2378) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 19       | 0.94          |
| (1,2178) | 1:26:A:MET:HE3   | 1:26:A:MET:HB3   | 4        | 0.94          |
| (1,2127) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 19       | 0.94          |
| (1,1971) | 1:43:A:ILE:HD12  | 1:91:A:GLU:H     | 13       | 0.94          |
| (1,1963) | 1:80:A:ILE:HD13  | 1:90:A:ILE:HA    | 2        | 0.94          |
| (1,3175) | 1:64:A:ALA:HB1   | 1:149:A:ARG:HD2  | 18       | 0.93          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD13  | 14       | 0.93          |
| (1,3115) | 1:131:A:ILE:HG12 | 1:70:A:ASN:HD21  | 13       | 0.93          |
| (1,3079) | 1:41:A:THR:HG23  | 1:41:A:THR:H     | 20       | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG22 | 1        | 0.93          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 7        | 0.93          |
| (1,2881) | 1:17:A:LEU:H     | 1:31:A:LYS:HB2   | 5        | 0.93          |
| (1,2815) | 1:134:A:MET:H    | 1:134:A:MET:HG3  | 1        | 0.93          |
| (1,2815) | 1:134:A:MET:H    | 1:134:A:MET:HG3  | 10       | 0.93          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD23  | 12       | 0.93          |
| (1,2332) | 1:17:A:LEU:H     | 1:13:A:ALA:HB2   | 17       | 0.93          |
| (1,3136) | 1:109:A:LYS:HG2  | 1:112:A:GLY:H    | 10       | 0.92          |
| (1,3079) | 1:41:A:THR:HG23  | 1:41:A:THR:H     | 8        | 0.92          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG22 | 15       | 0.92          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG21 | 17       | 0.92          |
| (1,2826) | 1:146:A:GLU:H    | 1:146:A:GLU:HG3  | 4        | 0.92          |
| (1,2815) | 1:134:A:MET:H    | 1:134:A:MET:HG2  | 8        | 0.92          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD13  | 10       | 0.91          |
| (1,3079) | 1:41:A:THR:HG23  | 1:41:A:THR:H     | 1        | 0.91          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG22 | 14       | 0.91          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG22 | 20       | 0.91          |
| (1,2815) | 1:134:A:MET:H    | 1:134:A:MET:HG3  | 6        | 0.91          |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD11 | 19       | 0.91          |
| (1,2481) | 1:103:A:ASN:H    | 1:96:A:ILE:HD13  | 10       | 0.91          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 14       | 0.9           |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 15       | 0.9           |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD22 | 13       | 0.9           |
| (1,2549) | 1:95:A:ASP:H     | 1:96:A:ILE:HG13  | 16       | 0.9           |
| (1,2178) | 1:26:A:MET:HE1   | 1:69:A:ASN:HB3   | 13       | 0.9           |
| (1,1967) | 1:80:A:ILE:HD12  | 1:54:A:VAL:HA    | 10       | 0.9           |
| (1,1956) | 1:96:A:ILE:HD13  | 1:97:A:ASP:H     | 5        | 0.9           |
| (1,3118) | 1:126:A:LEU:HD11 | 1:70:A:ASN:HD22  | 12       | 0.89          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG21 | 7        | 0.89          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG21 | 9        | 0.89          |
| (1,3031) | 1:131:A:ILE:H    | 1:131:A:ILE:HG22 | 10       | 0.89          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD11 | 2        | 0.89          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG12  | 6        | 0.89          |
| (1,2175) | 1:26:A:MET:HE3   | 1:16:A:SER:HA    | 8        | 0.89          |
| (1,1956) | 1:96:A:ILE:HD13  | 1:97:A:ASP:H     | 7        | 0.89          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD11  | 20       | 0.88          |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD21 | 11       | 0.88          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 18       | 0.88          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD13  | 2        | 0.88          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD12  | 6        | 0.88          |
| (1,2332) | 1:17:A:LEU:H     | 1:13:A:ALA:HB3   | 8        | 0.88          |
| (1,2274) | 1:116:A:LYS:HA   | 1:116:A:LYS:HE3  | 8        | 0.88          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2274) | 1:116:A:LYS:HA  | 1:116:A:LYS:HE3  | 12       | 0.88          |
| (1,2175) | 1:26:A:MET:HE1  | 1:16:A:SER:HA    | 10       | 0.88          |
| (1,2169) | 1:56:A:ILE:HG22 | 1:74:A:ARG:HB2   | 1        | 0.88          |
| (1,2074) | 1:11:A:ASP:HB3  | 1:36:A:ILE:HG12  | 14       | 0.88          |
| (1,1956) | 1:96:A:ILE:HD13 | 1:97:A:ASP:H     | 3        | 0.88          |
| (1,3159) | 1:15:A:LEU:HD22 | 1:136:A:GLN:H    | 13       | 0.87          |
| (1,3150) | 1:96:A:ILE:HB   | 1:36:A:ILE:HD11  | 19       | 0.87          |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD12  | 8        | 0.87          |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD13  | 13       | 0.87          |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD13  | 15       | 0.87          |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD12  | 20       | 0.87          |
| (1,2411) | 1:102:A:LEU:H   | 1:101:A:ILE:HD12 | 7        | 0.87          |
| (1,2411) | 1:102:A:LEU:H   | 1:96:A:ILE:HD11  | 11       | 0.87          |
| (1,2274) | 1:116:A:LYS:HA  | 1:116:A:LYS:HE3  | 5        | 0.87          |
| (1,3172) | 1:56:A:ILE:HD11 | 1:77:A:LEU:HA    | 8        | 0.86          |
| (1,3031) | 1:131:A:ILE:H   | 1:131:A:ILE:HG21 | 16       | 0.86          |
| (1,2916) | 1:96:A:ILE:H    | 1:102:A:LEU:HB2  | 15       | 0.86          |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD13  | 1        | 0.86          |
| (1,2761) | 1:30:A:ILE:H    | 1:17:A:LEU:HD13  | 17       | 0.86          |
| (1,2570) | 1:80:A:ILE:H    | 1:54:A:VAL:HG21  | 20       | 0.86          |
| (1,2481) | 1:103:A:ASN:H   | 1:96:A:ILE:HD12  | 16       | 0.86          |
| (1,2278) | 1:140:A:LYS:HB2 | 1:137:A:GLU:HG2  | 4        | 0.86          |
| (1,2224) | 1:44:A:PHE:H    | 1:43:A:ILE:HD12  | 15       | 0.86          |
| (1,2178) | 1:26:A:MET:HE1  | 1:69:A:ASN:HB3   | 16       | 0.86          |
| (1,3150) | 1:96:A:ILE:HB   | 1:36:A:ILE:HD11  | 16       | 0.85          |
| (1,3042) | 1:19:A:LEU:HD13 | 1:59:A:TYR:H     | 20       | 0.85          |
| (1,3031) | 1:131:A:ILE:H   | 1:131:A:ILE:HG23 | 18       | 0.85          |
| (1,3028) | 1:59:A:TYR:H    | 1:69:A:ASN:HB3   | 8        | 0.85          |
| (1,3028) | 1:59:A:TYR:H    | 1:69:A:ASN:HB3   | 10       | 0.85          |
| (1,2996) | 1:146:A:GLU:H   | 1:142:A:LYS:HG3  | 15       | 0.85          |
| (1,2815) | 1:134:A:MET:H   | 1:137:A:GLU:HG3  | 14       | 0.85          |
| (1,2684) | 1:158:A:LEU:H   | 1:90:A:ILE:HG12  | 13       | 0.85          |
| (1,2509) | 1:104:A:VAL:H   | 1:102:A:LEU:HD13 | 16       | 0.85          |
| (1,2274) | 1:116:A:LYS:HA  | 1:116:A:LYS:HE3  | 7        | 0.85          |
| (1,1956) | 1:96:A:ILE:HD13 | 1:97:A:ASP:H     | 18       | 0.85          |
| (1,3150) | 1:96:A:ILE:HB   | 1:36:A:ILE:HD12  | 11       | 0.84          |
| (1,3150) | 1:96:A:ILE:HB   | 1:36:A:ILE:HD11  | 17       | 0.84          |
| (1,3079) | 1:41:A:THR:HG21 | 1:41:A:THR:H     | 4        | 0.84          |
| (1,3045) | 1:14:A:PRO:HD3  | 1:13:A:ALA:H     | 8        | 0.84          |
| (1,2881) | 1:17:A:LEU:H    | 1:15:A:LEU:HB3   | 10       | 0.84          |
| (1,2684) | 1:158:A:LEU:H   | 1:90:A:ILE:HG13  | 5        | 0.84          |
| (1,2604) | 1:43:A:ILE:H    | 1:43:A:ILE:HG22  | 15       | 0.84          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD13 | 9        | 0.84          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD11  | 15       | 0.84          |
| (1,2274) | 1:116:A:LYS:HA   | 1:116:A:LYS:HE3  | 1        | 0.84          |
| (1,2188) | 1:80:A:ILE:HG21  | 1:46:A:THR:HA    | 17       | 0.84          |
| (1,2175) | 1:26:A:MET:HE1   | 1:16:A:SER:HA    | 14       | 0.84          |
| (1,3193) | 1:35:A:THR:H     | 1:36:A:ILE:HG12  | 8        | 0.83          |
| (1,3141) | 1:13:A:ALA:HB2   | 1:12:A:VAL:HB    | 19       | 0.83          |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD12 | 6        | 0.83          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 1        | 0.83          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD12  | 17       | 0.83          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 3        | 0.83          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD11  | 15       | 0.83          |
| (1,2224) | 1:44:A:PHE:H     | 1:43:A:ILE:HD12  | 1        | 0.83          |
| (1,2224) | 1:44:A:PHE:H     | 1:43:A:ILE:HD12  | 5        | 0.83          |
| (1,1956) | 1:96:A:ILE:HD11  | 1:97:A:ASP:H     | 19       | 0.83          |
| (1,1956) | 1:96:A:ILE:HD12  | 1:97:A:ASP:H     | 20       | 0.83          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD11  | 2        | 0.82          |
| (1,2747) | 1:11:A:ASP:H     | 1:10:A:LEU:HB3   | 1        | 0.82          |
| (1,2550) | 1:95:A:ASP:H     | 1:39:A:LYS:HB2   | 10       | 0.82          |
| (1,2378) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 10       | 0.82          |
| (1,2178) | 1:26:A:MET:HE3   | 1:69:A:ASN:HB3   | 11       | 0.82          |
| (1,2127) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 10       | 0.82          |
| (1,2725) | 1:38:A:THR:H     | 1:96:A:ILE:HG13  | 7        | 0.81          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 13       | 0.81          |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD12 | 6        | 0.81          |
| (1,2181) | 1:138:A:ALA:HB3  | 1:145:A:ASP:HB2  | 1        | 0.81          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD13  | 7        | 0.8           |
| (1,3079) | 1:93:A:THR:HG21  | 1:105:A:THR:H    | 15       | 0.8           |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG2   | 1        | 0.8           |
| (1,2826) | 1:146:A:GLU:H    | 1:146:A:GLU:HG3  | 16       | 0.8           |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 19       | 0.8           |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD13  | 5        | 0.8           |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD12 | 4        | 0.8           |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD13  | 3        | 0.8           |
| (1,2169) | 1:56:A:ILE:HG22  | 1:158:A:LEU:HG   | 19       | 0.8           |
| (1,1956) | 1:96:A:ILE:HD11  | 1:97:A:ASP:H     | 4        | 0.8           |
| (1,3174) | 1:70:A:ASN:HD21  | 1:126:A:LEU:HB2  | 11       | 0.79          |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HD1   | 20       | 0.79          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD12  | 14       | 0.79          |
| (1,2747) | 1:11:A:ASP:H     | 1:10:A:LEU:HB3   | 8        | 0.79          |
| (1,2378) | 1:158:A:LEU:HD22 | 1:54:A:VAL:HA    | 17       | 0.79          |
| (1,2175) | 1:26:A:MET:HE2   | 1:58:A:VAL:HA    | 13       | 0.79          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2127) | 1:158:A:LEU:HD22 | 1:54:A:VAL:HA    | 17       | 0.79          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD11  | 9        | 0.78          |
| (1,3079) | 1:93:A:THR:HG22  | 1:41:A:THR:H     | 12       | 0.78          |
| (1,3079) | 1:93:A:THR:HG22  | 1:105:A:THR:H    | 14       | 0.78          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 12       | 0.78          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD12  | 11       | 0.78          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG2  | 19       | 0.78          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG12  | 2        | 0.78          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 8        | 0.78          |
| (1,2550) | 1:95:A:ASP:H     | 1:39:A:LYS:HB2   | 17       | 0.78          |
| (1,2144) | 1:27:A:THR:HG22  | 1:42:A:GLN:HE22  | 7        | 0.78          |
| (1,1956) | 1:96:A:ILE:HD11  | 1:97:A:ASP:H     | 10       | 0.78          |
| (1,3175) | 1:64:A:ALA:HB2   | 1:149:A:ARG:HD3  | 9        | 0.77          |
| (1,3175) | 1:157:A:ALA:HB1  | 1:44:A:PHE:HB3   | 16       | 0.77          |
| (1,3141) | 1:13:A:ALA:HB3   | 1:12:A:VAL:HB    | 2        | 0.77          |
| (1,3141) | 1:13:A:ALA:HB2   | 1:12:A:VAL:HB    | 4        | 0.77          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 17       | 0.77          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 16       | 0.77          |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG21  | 18       | 0.77          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD11  | 13       | 0.77          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 9        | 0.76          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD13  | 13       | 0.76          |
| (1,3136) | 1:113:A:LYS:HG3  | 1:112:A:GLY:H    | 2        | 0.76          |
| (1,3079) | 1:93:A:THR:HG21  | 1:105:A:THR:H    | 11       | 0.76          |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD12 | 3        | 0.76          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 16       | 0.76          |
| (1,2996) | 1:146:A:GLU:H    | 1:143:A:ALA:HB3  | 19       | 0.76          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG21 | 16       | 0.76          |
| (1,2550) | 1:95:A:ASP:H     | 1:39:A:LYS:HB2   | 9        | 0.76          |
| (1,2481) | 1:103:A:ASN:H    | 1:30:A:ILE:HD13  | 1        | 0.76          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD21  | 5        | 0.76          |
| (1,2274) | 1:116:A:LYS:HA   | 1:116:A:LYS:HE3  | 3        | 0.76          |
| (1,2175) | 1:26:A:MET:HE2   | 1:16:A:SER:HA    | 17       | 0.76          |
| (1,2144) | 1:27:A:THR:HG21  | 1:42:A:GLN:HE22  | 14       | 0.76          |
| (1,1971) | 1:43:A:ILE:HD12  | 1:91:A:GLU:H     | 5        | 0.76          |
| (1,3141) | 1:13:A:ALA:HB3   | 1:12:A:VAL:HB    | 9        | 0.75          |
| (1,3079) | 1:93:A:THR:HG22  | 1:41:A:THR:H     | 19       | 0.75          |
| (1,3056) | 1:74:A:ARG:HB3   | 1:58:A:VAL:H     | 17       | 0.75          |
| (1,3042) | 1:19:A:LEU:HD13  | 1:59:A:TYR:H     | 7        | 0.75          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG23 | 15       | 0.75          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD12  | 2        | 0.75          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD21 | 8        | 0.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2550) | 1:95:A:ASP:H     | 1:39:A:LYS:HB2   | 7        | 0.75          |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD13 | 12       | 0.75          |
| (1,2509) | 1:104:A:VAL:H    | 1:102:A:LEU:HD13 | 13       | 0.75          |
| (1,2378) | 1:158:A:LEU:HD11 | 1:55:A:LEU:HA    | 3        | 0.75          |
| (1,2378) | 1:158:A:LEU:HD21 | 1:54:A:VAL:HA    | 11       | 0.75          |
| (1,2127) | 1:158:A:LEU:HD11 | 1:55:A:LEU:HA    | 3        | 0.75          |
| (1,2127) | 1:158:A:LEU:HD21 | 1:54:A:VAL:HA    | 11       | 0.75          |
| (1,2109) | 1:66:A:THR:HG23  | 1:27:A:THR:H     | 5        | 0.75          |
| (1,1980) | 1:30:A:ILE:HD11  | 1:94:A:PHE:HA    | 16       | 0.75          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 10       | 0.74          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 17       | 0.74          |
| (1,3141) | 1:13:A:ALA:HB2   | 1:32:A:ARG:HB2   | 3        | 0.74          |
| (1,3141) | 1:13:A:ALA:HB2   | 1:12:A:VAL:HB    | 14       | 0.74          |
| (1,3079) | 1:93:A:THR:HG23  | 1:41:A:THR:H     | 13       | 0.74          |
| (1,3053) | 1:102:A:LEU:HB3  | 1:104:A:VAL:H    | 11       | 0.74          |
| (1,2996) | 1:146:A:GLU:H    | 1:143:A:ALA:HB2  | 14       | 0.74          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD12  | 3        | 0.74          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD13  | 16       | 0.74          |
| (1,2750) | 1:11:A:ASP:H     | 1:12:A:VAL:HG23  | 5        | 0.74          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD13  | 13       | 0.74          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG12  | 14       | 0.74          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD12  | 9        | 0.74          |
| (1,2175) | 1:26:A:MET:HE3   | 1:16:A:SER:HA    | 16       | 0.74          |
| (1,1967) | 1:80:A:ILE:HD11  | 1:54:A:VAL:HA    | 3        | 0.74          |
| (1,1956) | 1:96:A:ILE:HD11  | 1:97:A:ASP:H     | 11       | 0.74          |
| (1,3174) | 1:70:A:ASN:HD21  | 1:126:A:LEU:HB2  | 1        | 0.73          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 11       | 0.73          |
| (1,2568) | 1:113:A:LYS:H    | 1:113:A:LYS:HG2  | 10       | 0.73          |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG23  | 17       | 0.73          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD11  | 10       | 0.73          |
| (1,2392) | 1:36:A:ILE:HD13  | 1:14:A:PRO:HD3   | 9        | 0.73          |
| (1,2256) | 1:94:A:PHE:HE2   | 1:19:A:LEU:HB2   | 8        | 0.73          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 4        | 0.72          |
| (1,2996) | 1:146:A:GLU:H    | 1:143:A:ALA:HB2  | 20       | 0.72          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 8        | 0.72          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD13  | 6        | 0.72          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 9        | 0.72          |
| (1,2392) | 1:36:A:ILE:HG22  | 1:14:A:PRO:HD3   | 4        | 0.72          |
| (1,1956) | 1:96:A:ILE:HD13  | 1:97:A:ASP:H     | 15       | 0.72          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 1        | 0.71          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD11  | 4        | 0.71          |
| (1,3150) | 1:96:A:ILE:HB    | 1:102:A:LEU:HD11 | 6        | 0.71          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG2   | 7        | 0.71          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD11  | 9        | 0.71          |
| (1,2698) | 1:127:A:SER:H    | 1:130:A:GLU:HG2  | 7        | 0.71          |
| (1,2481) | 1:103:A:ASN:H    | 1:30:A:ILE:HD13  | 8        | 0.71          |
| (1,2412) | 1:102:A:LEU:H    | 1:118:A:THR:HG21 | 19       | 0.71          |
| (1,2224) | 1:44:A:PHE:H     | 1:43:A:ILE:HD11  | 17       | 0.71          |
| (1,1956) | 1:96:A:ILE:HD13  | 1:97:A:ASP:H     | 8        | 0.71          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 12       | 0.7           |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 14       | 0.7           |
| (1,3177) | 1:26:A:MET:HE1   | 1:29:A:LEU:H     | 1        | 0.7           |
| (1,3053) | 1:102:A:LEU:HB3  | 1:104:A:VAL:H    | 4        | 0.7           |
| (1,2750) | 1:11:A:ASP:H     | 1:12:A:VAL:HG22  | 19       | 0.7           |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD12 | 18       | 0.7           |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 7        | 0.7           |
| (1,2582) | 1:51:A:GLN:H     | 1:85:A:ARG:HA    | 6        | 0.7           |
| (1,3141) | 1:13:A:ALA:HB3   | 1:12:A:VAL:HB    | 6        | 0.69          |
| (1,3042) | 1:19:A:LEU:HD11  | 1:59:A:TYR:H     | 18       | 0.69          |
| (1,3028) | 1:59:A:TYR:H     | 1:60:A:GLU:HG3   | 2        | 0.69          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 11       | 0.69          |
| (1,2996) | 1:146:A:GLU:H    | 1:143:A:ALA:HB2  | 9        | 0.69          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG21 | 6        | 0.69          |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HE2   | 4        | 0.69          |
| (1,2725) | 1:38:A:THR:H     | 1:96:A:ILE:HG22  | 18       | 0.69          |
| (1,2593) | 1:64:A:ALA:H     | 1:63:A:ARG:HD2   | 7        | 0.69          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG12  | 11       | 0.69          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD11  | 13       | 0.69          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD12  | 16       | 0.69          |
| (1,2075) | 1:130:A:GLU:H    | 1:130:A:GLU:HG2  | 8        | 0.69          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 7        | 0.68          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 13       | 0.68          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 19       | 0.68          |
| (1,3159) | 1:15:A:LEU:HD22  | 1:136:A:GLN:H    | 15       | 0.68          |
| (1,3159) | 1:15:A:LEU:HD23  | 1:131:A:ILE:H    | 17       | 0.68          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD13  | 5        | 0.68          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 19       | 0.68          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 6        | 0.68          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB2   | 13       | 0.68          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG3  | 16       | 0.68          |
| (1,2717) | 1:19:A:LEU:H     | 1:19:A:LEU:HD21  | 2        | 0.68          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG23  | 4        | 0.68          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD13  | 18       | 0.68          |
| (1,2381) | 1:104:A:VAL:HG12 | 1:117:A:ILE:HB   | 17       | 0.68          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2380) | 1:104:A:VAL:HG13 | 1:105:A:THR:HB   | 8        | 0.68          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD13  | 1        | 0.68          |
| (1,2188) | 1:80:A:ILE:HG21  | 1:53:A:GLY:HA2   | 1        | 0.68          |
| (1,2144) | 1:27:A:THR:HG23  | 1:156:A:ASN:HD22 | 13       | 0.68          |
| (1,1956) | 1:96:A:ILE:HD12  | 1:97:A:ASP:H     | 17       | 0.68          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 5        | 0.67          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB1   | 7        | 0.67          |
| (1,3141) | 1:13:A:ALA:HB3   | 1:12:A:VAL:HB    | 1        | 0.67          |
| (1,3136) | 1:113:A:LYS:HG2  | 1:112:A:GLY:H    | 9        | 0.67          |
| (1,3122) | 1:101:A:ILE:HG23 | 1:103:A:ASN:HD21 | 20       | 0.67          |
| (1,3028) | 1:59:A:TYR:H     | 1:60:A:GLU:HG3   | 3        | 0.67          |
| (1,2950) | 1:69:A:ASN:H     | 1:67:A:LYS:HG2   | 8        | 0.67          |
| (1,2873) | 1:103:A:ASN:HD21 | 1:101:A:ILE:HG23 | 20       | 0.67          |
| (1,2851) | 1:126:A:LEU:H    | 1:126:A:LEU:HD13 | 16       | 0.67          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD12  | 3        | 0.67          |
| (1,2178) | 1:26:A:MET:HE3   | 1:69:A:ASN:HB3   | 7        | 0.67          |
| (1,2175) | 1:26:A:MET:HE3   | 1:58:A:VAL:HA    | 1        | 0.67          |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 13       | 0.67          |
| (1,3141) | 1:13:A:ALA:HB1   | 1:12:A:VAL:HB    | 7        | 0.66          |
| (1,3141) | 1:13:A:ALA:HB3   | 1:32:A:ARG:HB3   | 11       | 0.66          |
| (1,3141) | 1:13:A:ALA:HB2   | 1:12:A:VAL:HB    | 12       | 0.66          |
| (1,3141) | 1:13:A:ALA:HB1   | 1:12:A:VAL:HB    | 15       | 0.66          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG22 | 14       | 0.66          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG22 | 15       | 0.66          |
| (1,2851) | 1:126:A:LEU:H    | 1:126:A:LEU:HD23 | 7        | 0.66          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD21 | 17       | 0.66          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 4        | 0.66          |
| (1,2549) | 1:95:A:ASP:H     | 1:102:A:LEU:HG   | 8        | 0.66          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 4        | 0.66          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD11  | 5        | 0.66          |
| (1,1956) | 1:96:A:ILE:HD13  | 1:97:A:ASP:H     | 16       | 0.66          |
| (1,3175) | 1:157:A:ALA:HB2  | 1:44:A:PHE:HB3   | 2        | 0.65          |
| (1,3159) | 1:15:A:LEU:HD21  | 1:136:A:GLN:H    | 10       | 0.65          |
| (1,3157) | 1:24:A:GLY:H     | 1:159:A:GLU:HG3  | 1        | 0.65          |
| (1,2916) | 1:96:A:ILE:H     | 1:102:A:LEU:HB2  | 6        | 0.65          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG23  | 10       | 0.65          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 2        | 0.65          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD12  | 14       | 0.64          |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD12 | 7        | 0.64          |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD11 | 19       | 0.64          |
| (1,3079) | 1:93:A:THR:HG21  | 1:41:A:THR:H     | 3        | 0.64          |
| (1,2862) | 1:86:A:GLY:H     | 1:45:A:THR:HG21  | 17       | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG2  | 16       | 0.64          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD13  | 6        | 0.64          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD13  | 14       | 0.64          |
| (1,1971) | 1:43:A:ILE:HD12  | 1:91:A:GLU:H     | 15       | 0.64          |
| (1,1956) | 1:96:A:ILE:HD11  | 1:97:A:ASP:H     | 13       | 0.64          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD13  | 8        | 0.63          |
| (1,3141) | 1:13:A:ALA:HB1   | 1:12:A:VAL:HB    | 10       | 0.63          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 5        | 0.63          |
| (1,3026) | 1:141:A:TYR:H    | 1:140:A:LYS:HD2  | 15       | 0.63          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG3  | 18       | 0.63          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD21 | 10       | 0.63          |
| (1,2380) | 1:104:A:VAL:HG13 | 1:105:A:THR:HB   | 6        | 0.63          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD13  | 12       | 0.63          |
| (1,3192) | 1:13:A:ALA:H     | 1:36:A:ILE:HG12  | 15       | 0.62          |
| (1,3141) | 1:13:A:ALA:HB3   | 1:12:A:VAL:HB    | 16       | 0.62          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 1        | 0.62          |
| (1,2916) | 1:96:A:ILE:H     | 1:102:A:LEU:HB2  | 11       | 0.62          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD22 | 1        | 0.62          |
| (1,2675) | 1:76:A:GLU:H     | 1:55:A:LEU:HD23  | 5        | 0.62          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 14       | 0.62          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD13  | 16       | 0.62          |
| (1,2380) | 1:104:A:VAL:HG11 | 1:105:A:THR:HB   | 3        | 0.62          |
| (1,2178) | 1:26:A:MET:HE1   | 1:69:A:ASN:HB3   | 5        | 0.62          |
| (1,2175) | 1:26:A:MET:HE3   | 1:58:A:VAL:HA    | 3        | 0.62          |
| (1,2020) | 1:72:A:LEU:HA    | 1:72:A:LEU:HD12  | 8        | 0.62          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 2        | 0.61          |
| (1,3174) | 1:70:A:ASN:HD21  | 1:126:A:LEU:HB3  | 4        | 0.61          |
| (1,3161) | 1:36:A:ILE:HD13  | 1:11:A:ASP:H     | 11       | 0.61          |
| (1,3125) | 1:75:A:PHE:HD1   | 1:117:A:ILE:HG21 | 2        | 0.61          |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD21 | 8        | 0.61          |
| (1,2979) | 1:110:A:SER:H    | 1:80:A:ILE:HG13  | 1        | 0.61          |
| (1,2979) | 1:110:A:SER:H    | 1:80:A:ILE:HG12  | 5        | 0.61          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG22 | 10       | 0.61          |
| (1,2844) | 1:118:A:THR:H    | 1:117:A:ILE:HB   | 1        | 0.61          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD22  | 18       | 0.61          |
| (1,2568) | 1:113:A:LYS:H    | 1:113:A:LYS:HG2  | 1        | 0.61          |
| (1,2222) | 1:158:A:LEU:HD21 | 1:56:A:ILE:HG22  | 16       | 0.61          |
| (1,2178) | 1:26:A:MET:HE3   | 1:69:A:ASN:HB3   | 9        | 0.61          |
| (1,2144) | 1:27:A:THR:HG22  | 1:156:A:ASN:HD22 | 18       | 0.61          |
| (1,1967) | 1:80:A:ILE:HD13  | 1:54:A:VAL:HA    | 8        | 0.61          |
| (1,1967) | 1:80:A:ILE:HD12  | 1:54:A:VAL:HA    | 14       | 0.61          |
| (1,3197) | 1:132:A:GLU:HB3  | 1:15:A:LEU:HD21  | 11       | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG22 | 17       | 0.6           |
| (1,2916) | 1:96:A:ILE:H     | 1:102:A:LEU:HB2  | 19       | 0.6           |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 15       | 0.6           |
| (1,2844) | 1:118:A:THR:H    | 1:117:A:ILE:HB   | 5        | 0.6           |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD12 | 14       | 0.6           |
| (1,2430) | 1:27:A:THR:H     | 1:19:A:LEU:HD13  | 8        | 0.6           |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD13  | 15       | 0.6           |
| (1,2387) | 1:29:A:LEU:HD22  | 1:92:A:VAL:HG11  | 16       | 0.6           |
| (1,2199) | 1:117:A:ILE:HD11 | 1:75:A:PHE:H     | 11       | 0.6           |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 15       | 0.6           |
| (1,1956) | 1:96:A:ILE:HD13  | 1:97:A:ASP:H     | 9        | 0.6           |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 11       | 0.59          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 9        | 0.59          |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG23  | 19       | 0.59          |
| (1,3141) | 1:13:A:ALA:HB3   | 1:12:A:VAL:HB    | 5        | 0.59          |
| (1,3079) | 1:93:A:THR:HG22  | 1:41:A:THR:H     | 2        | 0.59          |
| (1,3052) | 1:29:A:LEU:HD21  | 1:42:A:GLN:H     | 13       | 0.59          |
| (1,2967) | 1:99:A:ASN:H     | 1:36:A:ILE:HD13  | 8        | 0.59          |
| (1,2896) | 1:16:A:SER:H     | 1:32:A:ARG:HB3   | 17       | 0.59          |
| (1,2862) | 1:86:A:GLY:H     | 1:85:A:ARG:HB3   | 16       | 0.59          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD22 | 6        | 0.59          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG21  | 1        | 0.59          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG13  | 9        | 0.59          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG13  | 11       | 0.59          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD12  | 10       | 0.59          |
| (1,2109) | 1:66:A:THR:HG21  | 1:27:A:THR:H     | 3        | 0.59          |
| (1,2109) | 1:66:A:THR:HG21  | 1:27:A:THR:H     | 10       | 0.59          |
| (1,1956) | 1:96:A:ILE:HD11  | 1:97:A:ASP:H     | 2        | 0.59          |
| (1,3159) | 1:15:A:LEU:HD23  | 1:136:A:GLN:H    | 20       | 0.58          |
| (1,3079) | 1:93:A:THR:HG22  | 1:105:A:THR:H    | 18       | 0.58          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 15       | 0.58          |
| (1,3026) | 1:141:A:TYR:H    | 1:138:A:ALA:HB2  | 17       | 0.58          |
| (1,2996) | 1:146:A:GLU:H    | 1:142:A:LYS:HG3  | 2        | 0.58          |
| (1,2996) | 1:146:A:GLU:H    | 1:143:A:ALA:HB1  | 10       | 0.58          |
| (1,2967) | 1:99:A:ASN:H     | 1:36:A:ILE:HD13  | 15       | 0.58          |
| (1,2916) | 1:96:A:ILE:H     | 1:102:A:LEU:HB2  | 12       | 0.58          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 14       | 0.58          |
| (1,2748) | 1:11:A:ASP:H     | 1:36:A:ILE:HG12  | 10       | 0.58          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD22 | 19       | 0.58          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 17       | 0.58          |
| (1,2174) | 1:26:A:MET:HE2   | 1:59:A:TYR:H     | 10       | 0.58          |
| (1,3141) | 1:13:A:ALA:HB2   | 1:12:A:VAL:HB    | 13       | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3141) | 1:13:A:ALA:HB3   | 1:12:A:VAL:HB    | 17       | 0.57          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 4        | 0.57          |
| (1,3026) | 1:141:A:TYR:H    | 1:138:A:ALA:HB3  | 10       | 0.57          |
| (1,3026) | 1:141:A:TYR:H    | 1:138:A:ALA:HB3  | 19       | 0.57          |
| (1,2967) | 1:99:A:ASN:H     | 1:36:A:ILE:HD13  | 7        | 0.57          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG3   | 8        | 0.57          |
| (1,2844) | 1:118:A:THR:H    | 1:117:A:ILE:HB   | 17       | 0.57          |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HE1   | 16       | 0.57          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG22  | 19       | 0.57          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD13  | 1        | 0.57          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 6        | 0.57          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG21  | 11       | 0.57          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD11  | 5        | 0.57          |
| (1,2412) | 1:102:A:LEU:H    | 1:118:A:THR:HG22 | 1        | 0.57          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD13  | 3        | 0.57          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 10       | 0.57          |
| (1,2387) | 1:29:A:LEU:HD22  | 1:92:A:VAL:HG11  | 13       | 0.57          |
| (1,2274) | 1:115:A:ASN:HA   | 1:116:A:LYS:HE2  | 17       | 0.57          |
| (1,2181) | 1:138:A:ALA:HB1  | 1:145:A:ASP:HB2  | 6        | 0.57          |
| (1,2109) | 1:66:A:THR:HG21  | 1:27:A:THR:H     | 2        | 0.57          |
| (1,3192) | 1:13:A:ALA:H     | 1:36:A:ILE:HG12  | 8        | 0.56          |
| (1,3053) | 1:149:A:ARG:HB2  | 1:26:A:MET:H     | 5        | 0.56          |
| (1,2996) | 1:146:A:GLU:H    | 1:142:A:LYS:HG3  | 17       | 0.56          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG22 | 20       | 0.56          |
| (1,2950) | 1:69:A:ASN:H     | 1:67:A:LYS:HG3   | 3        | 0.56          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG22 | 1        | 0.56          |
| (1,2817) | 1:134:A:MET:H    | 1:131:A:ILE:HG23 | 12       | 0.56          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD13  | 5        | 0.56          |
| (1,2747) | 1:11:A:ASP:H     | 1:10:A:LEU:HB3   | 15       | 0.56          |
| (1,2699) | 1:127:A:SER:H    | 1:131:A:ILE:HD12 | 12       | 0.56          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD13 | 8        | 0.56          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG21  | 18       | 0.56          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 1        | 0.56          |
| (1,2556) | 1:40:A:GLN:H     | 1:30:A:ILE:HG12  | 8        | 0.56          |
| (1,2324) | 1:139:A:GLU:HG2  | 1:142:A:LYS:HG2  | 15       | 0.56          |
| (1,2144) | 1:27:A:THR:HG23  | 1:42:A:GLN:HE22  | 10       | 0.56          |
| (1,1956) | 1:96:A:ILE:HD13  | 1:97:A:ASP:H     | 14       | 0.56          |
| (1,3161) | 1:36:A:ILE:HD13  | 1:13:A:ALA:H     | 20       | 0.55          |
| (1,3118) | 1:126:A:LEU:HD12 | 1:70:A:ASN:HD21  | 16       | 0.55          |
| (1,3079) | 1:93:A:THR:HG21  | 1:41:A:THR:H     | 5        | 0.55          |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H     | 1        | 0.55          |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD21 | 12       | 0.55          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2916) | 1:96:A:ILE:H     | 1:102:A:LEU:HB2  | 4        | 0.55          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG3   | 14       | 0.55          |
| (1,2716) | 1:19:A:LEU:H     | 1:29:A:LEU:HB2   | 8        | 0.55          |
| (1,2699) | 1:127:A:SER:H    | 1:131:A:ILE:HD11 | 11       | 0.55          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 15       | 0.55          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 6        | 0.55          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 12       | 0.55          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 8        | 0.55          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD12 | 4        | 0.55          |
| (1,2378) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 2        | 0.55          |
| (1,2378) | 1:158:A:LEU:HD21 | 1:55:A:LEU:HA    | 9        | 0.55          |
| (1,2356) | 1:32:A:ARG:HA    | 1:15:A:LEU:HD23  | 13       | 0.55          |
| (1,2200) | 1:96:A:ILE:HD12  | 1:38:A:THR:H     | 19       | 0.55          |
| (1,2169) | 1:56:A:ILE:HG22  | 1:74:A:ARG:HB2   | 4        | 0.55          |
| (1,2127) | 1:158:A:LEU:HD11 | 1:54:A:VAL:HA    | 2        | 0.55          |
| (1,2127) | 1:158:A:LEU:HD21 | 1:55:A:LEU:HA    | 9        | 0.55          |
| (1,3177) | 1:26:A:MET:HE2   | 1:29:A:LEU:H     | 9        | 0.54          |
| (1,3177) | 1:26:A:MET:HE3   | 1:29:A:LEU:H     | 20       | 0.54          |
| (1,3079) | 1:93:A:THR:HG22  | 1:105:A:THR:H    | 7        | 0.54          |
| (1,3045) | 1:53:A:GLY:HA2   | 1:77:A:LEU:H     | 9        | 0.54          |
| (1,2937) | 1:65:A:MET:H     | 1:63:A:ARG:HB2   | 11       | 0.54          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG3   | 16       | 0.54          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG22  | 20       | 0.54          |
| (1,1963) | 1:80:A:ILE:HD13  | 1:77:A:LEU:HA    | 11       | 0.54          |
| (1,3175) | 1:157:A:ALA:HB2  | 1:44:A:PHE:HB3   | 7        | 0.53          |
| (1,3151) | 1:38:A:THR:HB    | 1:96:A:ILE:HG21  | 9        | 0.53          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB2   | 5        | 0.53          |
| (1,3011) | 1:157:A:ALA:H    | 1:158:A:LEU:HG   | 4        | 0.53          |
| (1,2983) | 1:116:A:LYS:H    | 1:105:A:THR:HG22 | 15       | 0.53          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB3   | 12       | 0.53          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB3   | 16       | 0.53          |
| (1,2844) | 1:118:A:THR:H    | 1:116:A:LYS:HD2  | 3        | 0.53          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD11 | 20       | 0.53          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 3        | 0.53          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 15       | 0.53          |
| (1,2550) | 1:95:A:ASP:H     | 1:39:A:LYS:HB2   | 19       | 0.53          |
| (1,2420) | 1:119:A:ILE:H    | 1:117:A:ILE:HG22 | 5        | 0.53          |
| (1,2380) | 1:104:A:VAL:HG13 | 1:105:A:THR:HB   | 1        | 0.53          |
| (1,2380) | 1:104:A:VAL:HG11 | 1:105:A:THR:HB   | 10       | 0.53          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD11  | 18       | 0.53          |
| (1,2220) | 1:143:A:ALA:HB2  | 1:146:A:GLU:HB2  | 8        | 0.53          |
| (1,2169) | 1:56:A:ILE:HG23  | 1:58:A:VAL:HB    | 16       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2144) | 1:27:A:THR:HG23  | 1:42:A:GLN:HE22  | 12       | 0.53          |
| (1,1956) | 1:96:A:ILE:HD12  | 1:97:A:ASP:H     | 1        | 0.53          |
| (1,3161) | 1:36:A:ILE:HD13  | 1:13:A:ALA:H     | 9        | 0.52          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG23 | 8        | 0.52          |
| (1,2807) | 1:132:A:GLU:H    | 1:132:A:GLU:HG3  | 18       | 0.52          |
| (1,2806) | 1:132:A:GLU:H    | 1:132:A:GLU:HG3  | 18       | 0.52          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG2  | 11       | 0.52          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG3  | 15       | 0.52          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG12  | 2        | 0.52          |
| (1,2550) | 1:95:A:ASP:H     | 1:39:A:LYS:HB2   | 5        | 0.52          |
| (1,2412) | 1:102:A:LEU:H    | 1:118:A:THR:HG21 | 18       | 0.52          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 13       | 0.52          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG23  | 8        | 0.52          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG22  | 10       | 0.52          |
| (1,2039) | 1:74:A:ARG:HA    | 1:55:A:LEU:HD13  | 20       | 0.52          |
| (1,3160) | 1:143:A:ALA:HA   | 1:142:A:LYS:HB2  | 9        | 0.51          |
| (1,3151) | 1:13:A:ALA:HA    | 1:96:A:ILE:HG21  | 11       | 0.51          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD11  | 3        | 0.51          |
| (1,2972) | 1:104:A:VAL:H    | 1:117:A:ILE:HG12 | 8        | 0.51          |
| (1,2946) | 1:68:A:ASP:H     | 1:69:A:ASN:HA    | 7        | 0.51          |
| (1,2884) | 1:133:A:ARG:H    | 1:133:A:ARG:HG2  | 13       | 0.51          |
| (1,2851) | 1:126:A:LEU:H    | 1:126:A:LEU:HD22 | 3        | 0.51          |
| (1,2747) | 1:11:A:ASP:H     | 1:10:A:LEU:HG    | 3        | 0.51          |
| (1,2716) | 1:19:A:LEU:H     | 1:29:A:LEU:HB2   | 20       | 0.51          |
| (1,2549) | 1:95:A:ASP:H     | 1:96:A:ILE:HG13  | 20       | 0.51          |
| (1,2544) | 1:114:A:ALA:H    | 1:113:A:LYS:HB2  | 1        | 0.51          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 19       | 0.51          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG22  | 17       | 0.51          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG21  | 19       | 0.51          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 12       | 0.51          |
| (1,2144) | 1:27:A:THR:HG21  | 1:42:A:GLN:HE21  | 8        | 0.51          |
| (1,3122) | 1:101:A:ILE:HG21 | 1:103:A:ASN:HD21 | 16       | 0.5           |
| (1,3092) | 1:30:A:ILE:HG13  | 1:30:A:ILE:H     | 18       | 0.5           |
| (1,3022) | 1:130:A:GLU:H    | 1:133:A:ARG:HG3  | 12       | 0.5           |
| (1,2979) | 1:110:A:SER:H    | 1:80:A:ILE:HG12  | 7        | 0.5           |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG22 | 10       | 0.5           |
| (1,2950) | 1:69:A:ASN:H     | 1:67:A:LYS:HG2   | 6        | 0.5           |
| (1,2884) | 1:133:A:ARG:H    | 1:133:A:ARG:HG3  | 19       | 0.5           |
| (1,2873) | 1:103:A:ASN:HD21 | 1:101:A:ILE:HG21 | 16       | 0.5           |
| (1,2842) | 1:140:A:LYS:H    | 1:139:A:GLU:HB2  | 4        | 0.5           |
| (1,2725) | 1:38:A:THR:H     | 1:96:A:ILE:HG13  | 5        | 0.5           |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB3   | 13       | 0.5           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD23 | 7        | 0.5           |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 7        | 0.5           |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD13 | 7        | 0.5           |
| (1,2412) | 1:102:A:LEU:H    | 1:118:A:THR:HG22 | 15       | 0.5           |
| (1,2380) | 1:104:A:VAL:HG11 | 1:105:A:THR:HB   | 20       | 0.5           |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD13  | 19       | 0.5           |
| (1,2324) | 1:139:A:GLU:HG2  | 1:142:A:LYS:HG2  | 9        | 0.5           |
| (1,1963) | 1:80:A:ILE:HD12  | 1:77:A:LEU:HA    | 14       | 0.5           |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 14       | 0.49          |
| (1,3028) | 1:59:A:TYR:H     | 1:60:A:GLU:HG3   | 5        | 0.49          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG23 | 13       | 0.49          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB2   | 12       | 0.49          |
| (1,2844) | 1:118:A:THR:H    | 1:116:A:LYS:HD2  | 7        | 0.49          |
| (1,2844) | 1:118:A:THR:H    | 1:117:A:ILE:HB   | 18       | 0.49          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD21  | 12       | 0.49          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB2   | 11       | 0.49          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB3   | 15       | 0.49          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD23 | 16       | 0.49          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 5        | 0.49          |
| (1,2550) | 1:95:A:ASP:H     | 1:39:A:LYS:HB2   | 16       | 0.49          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG23  | 11       | 0.49          |
| (1,2380) | 1:104:A:VAL:HG11 | 1:105:A:THR:HB   | 5        | 0.49          |
| (1,2181) | 1:138:A:ALA:HB2  | 1:134:A:MET:HB3  | 10       | 0.49          |
| (1,2178) | 1:26:A:MET:HE3   | 1:69:A:ASN:HB3   | 12       | 0.49          |
| (1,2175) | 1:26:A:MET:HE1   | 1:58:A:VAL:HA    | 12       | 0.49          |
| (1,2169) | 1:56:A:ILE:HG21  | 1:58:A:VAL:HB    | 5        | 0.49          |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 4        | 0.49          |
| (1,1963) | 1:80:A:ILE:HD11  | 1:52:A:PRO:HA    | 12       | 0.49          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 9        | 0.48          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 17       | 0.48          |
| (1,3151) | 1:13:A:ALA:HA    | 1:96:A:ILE:HG22  | 4        | 0.48          |
| (1,3141) | 1:13:A:ALA:HB2   | 1:12:A:VAL:HB    | 20       | 0.48          |
| (1,3065) | 1:92:A:VAL:HG13  | 1:93:A:THR:H     | 8        | 0.48          |
| (1,2996) | 1:146:A:GLU:H    | 1:143:A:ALA:HB3  | 13       | 0.48          |
| (1,2967) | 1:99:A:ASN:H     | 1:36:A:ILE:HD13  | 5        | 0.48          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG21 | 11       | 0.48          |
| (1,2748) | 1:11:A:ASP:H     | 1:36:A:ILE:HG12  | 1        | 0.48          |
| (1,2725) | 1:38:A:THR:H     | 1:96:A:ILE:HG22  | 6        | 0.48          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG21  | 4        | 0.48          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 4        | 0.48          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 11       | 0.48          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG22  | 4        | 0.48          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG13  | 14       | 0.48          |
| (1,2420) | 1:119:A:ILE:H    | 1:101:A:ILE:HG22 | 17       | 0.48          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 9        | 0.48          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 15       | 0.48          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 17       | 0.48          |
| (1,2392) | 1:36:A:ILE:HD12  | 1:14:A:PRO:HD3   | 5        | 0.48          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 9        | 0.48          |
| (1,2378) | 1:158:A:LEU:HD12 | 1:54:A:VAL:HA    | 4        | 0.48          |
| (1,2216) | 1:13:A:ALA:HB3   | 1:32:A:ARG:HB2   | 5        | 0.48          |
| (1,2127) | 1:158:A:LEU:HD12 | 1:54:A:VAL:HA    | 4        | 0.48          |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 9        | 0.48          |
| (1,1963) | 1:80:A:ILE:HD11  | 1:52:A:PRO:HA    | 7        | 0.48          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB2   | 18       | 0.47          |
| (1,3125) | 1:75:A:PHE:HD2   | 1:117:A:ILE:HG22 | 11       | 0.47          |
| (1,3069) | 1:75:A:PHE:HE1   | 1:115:A:ASN:H    | 12       | 0.47          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG23 | 14       | 0.47          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB3   | 10       | 0.47          |
| (1,2931) | 1:62:A:GLU:H     | 1:62:A:GLU:HG3   | 9        | 0.47          |
| (1,2909) | 1:147:A:VAL:H    | 1:146:A:GLU:HB2  | 11       | 0.47          |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HE1   | 6        | 0.47          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD21  | 15       | 0.47          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB3   | 16       | 0.47          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD22 | 4        | 0.47          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG3  | 13       | 0.47          |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG21  | 10       | 0.47          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG11  | 10       | 0.47          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG12  | 17       | 0.47          |
| (1,2501) | 1:31:A:LYS:H     | 1:13:A:ALA:HB3   | 16       | 0.47          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD11 | 2        | 0.47          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD11 | 18       | 0.47          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD11  | 19       | 0.47          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 5        | 0.47          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 14       | 0.47          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 20       | 0.47          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 2        | 0.47          |
| (1,2175) | 1:26:A:MET:HE2   | 1:16:A:SER:HA    | 19       | 0.47          |
| (1,2109) | 1:66:A:THR:HG21  | 1:27:A:THR:H     | 17       | 0.47          |
| (1,3160) | 1:143:A:ALA:HA   | 1:142:A:LYS:HB3  | 11       | 0.46          |
| (1,3160) | 1:143:A:ALA:HA   | 1:142:A:LYS:HB3  | 12       | 0.46          |
| (1,3157) | 1:24:A:GLY:H     | 1:159:A:GLU:HG3  | 13       | 0.46          |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD13 | 14       | 0.46          |
| (1,3026) | 1:141:A:TYR:H    | 1:140:A:LYS:HD3  | 5        | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG22 | 2        | 0.46          |
| (1,2851) | 1:126:A:LEU:H    | 1:126:A:LEU:HD21 | 19       | 0.46          |
| (1,2725) | 1:38:A:THR:H     | 1:96:A:ILE:HG13  | 9        | 0.46          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG21  | 1        | 0.46          |
| (1,2567) | 1:113:A:LYS:H    | 1:114:A:ALA:HB2  | 9        | 0.46          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 12       | 0.46          |
| (1,2539) | 1:32:A:ARG:H     | 1:31:A:LYS:HB3   | 9        | 0.46          |
| (1,2530) | 1:90:A:ILE:H     | 1:43:A:ILE:HG21  | 16       | 0.46          |
| (1,2516) | 1:96:A:ILE:H     | 1:39:A:LYS:HB2   | 12       | 0.46          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 2        | 0.46          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 3        | 0.46          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 6        | 0.46          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 8        | 0.46          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 16       | 0.46          |
| (1,2109) | 1:66:A:THR:HG23  | 1:27:A:THR:H     | 11       | 0.46          |
| (1,3173) | 1:70:A:ASN:HD22  | 1:15:A:LEU:HB3   | 7        | 0.45          |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD21 | 1        | 0.45          |
| (1,3069) | 1:75:A:PHE:HD2   | 1:75:A:PHE:H     | 17       | 0.45          |
| (1,3052) | 1:29:A:LEU:HD21  | 1:42:A:GLN:H     | 1        | 0.45          |
| (1,3052) | 1:29:A:LEU:HD22  | 1:42:A:GLN:H     | 11       | 0.45          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG22 | 2        | 0.45          |
| (1,2967) | 1:99:A:ASN:H     | 1:36:A:ILE:HD11  | 6        | 0.45          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG3   | 5        | 0.45          |
| (1,2784) | 1:150:A:GLU:H    | 1:150:A:GLU:HG2  | 18       | 0.45          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD22  | 16       | 0.45          |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG22  | 6        | 0.45          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG13  | 16       | 0.45          |
| (1,2447) | 1:97:A:ASP:H     | 1:96:A:ILE:HD12  | 6        | 0.45          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD12  | 16       | 0.45          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 11       | 0.45          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG22  | 1        | 0.45          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG22  | 6        | 0.45          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 11       | 0.45          |
| (1,2380) | 1:104:A:VAL:HG11 | 1:105:A:THR:HB   | 15       | 0.45          |
| (1,2380) | 1:104:A:VAL:HG11 | 1:105:A:THR:HB   | 18       | 0.45          |
| (1,2379) | 1:158:A:LEU:HD23 | 1:21:A:THR:H     | 19       | 0.45          |
| (1,2316) | 1:15:A:LEU:HD11  | 1:14:A:PRO:HG2   | 17       | 0.45          |
| (1,2020) | 1:72:A:LEU:HA    | 1:72:A:LEU:HD13  | 16       | 0.45          |
| (1,1956) | 1:96:A:ILE:HD12  | 1:97:A:ASP:H     | 6        | 0.45          |
| (1,3125) | 1:75:A:PHE:HD2   | 1:117:A:ILE:HG23 | 12       | 0.44          |
| (1,3079) | 1:93:A:THR:HG21  | 1:41:A:THR:H     | 16       | 0.44          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB3   | 3        | 0.44          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB2   | 19       | 0.44          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG3   | 10       | 0.44          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 16       | 0.44          |
| (1,2824) | 1:146:A:GLU:H    | 1:142:A:LYS:HA   | 18       | 0.44          |
| (1,2817) | 1:134:A:MET:H    | 1:15:A:LEU:HD22  | 17       | 0.44          |
| (1,2776) | 1:20:A:GLU:H     | 1:66:A:THR:HG21  | 15       | 0.44          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD22  | 13       | 0.44          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD23  | 17       | 0.44          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB2   | 2        | 0.44          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG22  | 12       | 0.44          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG12  | 19       | 0.44          |
| (1,2530) | 1:90:A:ILE:H     | 1:43:A:ILE:HG22  | 2        | 0.44          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD12  | 11       | 0.44          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 19       | 0.44          |
| (1,2216) | 1:13:A:ALA:HB1   | 1:32:A:ARG:HB3   | 7        | 0.44          |
| (1,3028) | 1:59:A:TYR:H     | 1:69:A:ASN:HB3   | 4        | 0.43          |
| (1,3017) | 1:12:A:VAL:H     | 1:14:A:PRO:HD3   | 16       | 0.43          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG21 | 3        | 0.43          |
| (1,2950) | 1:69:A:ASN:H     | 1:67:A:LYS:HG3   | 4        | 0.43          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB3   | 4        | 0.43          |
| (1,2909) | 1:147:A:VAL:H    | 1:146:A:GLU:HB2  | 3        | 0.43          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG23 | 6        | 0.43          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG2  | 5        | 0.43          |
| (1,2698) | 1:127:A:SER:H    | 1:130:A:GLU:HB2  | 1        | 0.43          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG23  | 19       | 0.43          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG13  | 2        | 0.43          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG21 | 4        | 0.43          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 12       | 0.43          |
| (1,2381) | 1:104:A:VAL:HG13 | 1:19:A:LEU:HG    | 9        | 0.43          |
| (1,2381) | 1:104:A:VAL:HG13 | 1:19:A:LEU:HG    | 13       | 0.43          |
| (1,2178) | 1:26:A:MET:HE2   | 1:69:A:ASN:HB3   | 3        | 0.43          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 4        | 0.42          |
| (1,3159) | 1:15:A:LEU:HD12  | 1:136:A:GLN:H    | 11       | 0.42          |
| (1,3157) | 1:24:A:GLY:H     | 1:159:A:GLU:HG3  | 6        | 0.42          |
| (1,3156) | 1:70:A:ASN:H     | 1:126:A:LEU:HD12 | 13       | 0.42          |
| (1,3092) | 1:30:A:ILE:HG13  | 1:30:A:ILE:H     | 7        | 0.42          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 2        | 0.42          |
| (1,2979) | 1:110:A:SER:H    | 1:107:A:THR:HG22 | 9        | 0.42          |
| (1,2979) | 1:110:A:SER:H    | 1:80:A:ILE:HG13  | 19       | 0.42          |
| (1,2896) | 1:16:A:SER:H     | 1:32:A:ARG:HB3   | 20       | 0.42          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG23 | 3        | 0.42          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG22 | 5        | 0.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 2        | 0.42          |
| (1,2817) | 1:134:A:MET:H    | 1:131:A:ILE:HG23 | 6        | 0.42          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG2  | 13       | 0.42          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG3  | 20       | 0.42          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 10       | 0.42          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG21  | 14       | 0.42          |
| (1,2582) | 1:51:A:GLN:H     | 1:48:A:SER:HB2   | 8        | 0.42          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD11  | 12       | 0.42          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 18       | 0.42          |
| (1,2344) | 1:253:A:ILE:HA   | 1:254:A:GLU:HG2  | 16       | 0.42          |
| (1,1967) | 1:80:A:ILE:HD13  | 1:54:A:VAL:HA    | 4        | 0.42          |
| (1,3177) | 1:26:A:MET:HE1   | 1:29:A:LEU:H     | 3        | 0.41          |
| (1,3174) | 1:70:A:ASN:HD21  | 1:15:A:LEU:HB2   | 2        | 0.41          |
| (1,3161) | 1:36:A:ILE:HD12  | 1:13:A:ALA:H     | 18       | 0.41          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 1        | 0.41          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB2   | 15       | 0.41          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB2   | 18       | 0.41          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG21 | 7        | 0.41          |
| (1,2868) | 1:12:A:VAL:H     | 1:12:A:VAL:HB    | 2        | 0.41          |
| (1,2868) | 1:12:A:VAL:H     | 1:12:A:VAL:HB    | 5        | 0.41          |
| (1,2748) | 1:11:A:ASP:H     | 1:36:A:ILE:HG12  | 7        | 0.41          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD13 | 1        | 0.41          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD23 | 9        | 0.41          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD13  | 6        | 0.41          |
| (1,2597) | 1:142:A:LYS:H    | 1:142:A:LYS:HG2  | 19       | 0.41          |
| (1,2539) | 1:32:A:ARG:H     | 1:31:A:LYS:HB2   | 13       | 0.41          |
| (1,2530) | 1:90:A:ILE:H     | 1:43:A:ILE:HG22  | 4        | 0.41          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD11 | 15       | 0.41          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 13       | 0.41          |
| (1,2378) | 1:158:A:LEU:HD23 | 1:55:A:LEU:HA    | 7        | 0.41          |
| (1,2200) | 1:96:A:ILE:HD13  | 1:38:A:THR:H     | 12       | 0.41          |
| (1,2175) | 1:26:A:MET:HE2   | 1:58:A:VAL:HA    | 20       | 0.41          |
| (1,2127) | 1:158:A:LEU:HD23 | 1:55:A:LEU:HA    | 7        | 0.41          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 15       | 0.4           |
| (1,3173) | 1:70:A:ASN:HD22  | 1:126:A:LEU:HB2  | 11       | 0.4           |
| (1,3161) | 1:36:A:ILE:HD12  | 1:11:A:ASP:H     | 4        | 0.4           |
| (1,3161) | 1:36:A:ILE:HD13  | 1:13:A:ALA:H     | 16       | 0.4           |
| (1,3154) | 1:46:A:THR:H     | 1:80:A:ILE:HG22  | 8        | 0.4           |
| (1,3118) | 1:131:A:ILE:HD12 | 1:70:A:ASN:HD22  | 17       | 0.4           |
| (1,3117) | 1:126:A:LEU:HB2  | 1:70:A:ASN:HD22  | 11       | 0.4           |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H     | 18       | 0.4           |
| (1,3001) | 1:157:A:ALA:H    | 1:22:A:ALA:H     | 20       | 0.4           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB3   | 14       | 0.4           |
| (1,2921) | 1:48:A:SER:H     | 1:157:A:ALA:HB2  | 9        | 0.4           |
| (1,2909) | 1:147:A:VAL:H    | 1:146:A:GLU:HB3  | 12       | 0.4           |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG21 | 4        | 0.4           |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 7        | 0.4           |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 11       | 0.4           |
| (1,2881) | 1:17:A:LEU:H     | 1:31:A:LYS:HB3   | 17       | 0.4           |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 19       | 0.4           |
| (1,2851) | 1:126:A:LEU:H    | 1:131:A:ILE:HD13 | 6        | 0.4           |
| (1,2817) | 1:134:A:MET:H    | 1:131:A:ILE:HG23 | 8        | 0.4           |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD13  | 10       | 0.4           |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG2  | 17       | 0.4           |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG21  | 15       | 0.4           |
| (1,2698) | 1:127:A:SER:H    | 1:130:A:GLU:HB2  | 3        | 0.4           |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD11 | 1        | 0.4           |
| (1,2378) | 1:158:A:LEU:HD13 | 1:54:A:VAL:HA    | 5        | 0.4           |
| (1,2175) | 1:26:A:MET:HE2   | 1:16:A:SER:HA    | 9        | 0.4           |
| (1,2127) | 1:158:A:LEU:HD13 | 1:54:A:VAL:HA    | 5        | 0.4           |
| (1,3175) | 1:157:A:ALA:HB1  | 1:44:A:PHE:HB3   | 14       | 0.39          |
| (1,3174) | 1:70:A:ASN:HD21  | 1:15:A:LEU:HB2   | 12       | 0.39          |
| (1,3173) | 1:70:A:ASN:HD22  | 1:126:A:LEU:HB2  | 14       | 0.39          |
| (1,3125) | 1:75:A:PHE:HD2   | 1:117:A:ILE:HG23 | 20       | 0.39          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 6        | 0.39          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 18       | 0.39          |
| (1,2996) | 1:146:A:GLU:H    | 1:142:A:LYS:HG2  | 16       | 0.39          |
| (1,2979) | 1:110:A:SER:H    | 1:80:A:ILE:HG13  | 8        | 0.39          |
| (1,2921) | 1:48:A:SER:H     | 1:85:A:ARG:HG3   | 16       | 0.39          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG3   | 17       | 0.39          |
| (1,2868) | 1:12:A:VAL:H     | 1:12:A:VAL:HB    | 4        | 0.39          |
| (1,2868) | 1:12:A:VAL:H     | 1:12:A:VAL:HB    | 8        | 0.39          |
| (1,2817) | 1:134:A:MET:H    | 1:131:A:ILE:HG22 | 14       | 0.39          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD22  | 1        | 0.39          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB2   | 18       | 0.39          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD13 | 5        | 0.39          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG22  | 5        | 0.39          |
| (1,2420) | 1:119:A:ILE:H    | 1:101:A:ILE:HG22 | 6        | 0.39          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD11  | 19       | 0.39          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG21  | 9        | 0.39          |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 20       | 0.39          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22  | 6        | 0.38          |
| (1,3189) | 1:12:A:VAL:HG11  | 1:33:A:ASN:HA    | 8        | 0.38          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 14       | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3160) | 1:143:A:ALA:HA   | 1:142:A:LYS:HB3  | 3        | 0.38          |
| (1,3151) | 1:13:A:ALA:HA    | 1:96:A:ILE:HG21  | 5        | 0.38          |
| (1,3150) | 1:96:A:ILE:HB    | 1:36:A:ILE:HD13  | 15       | 0.38          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 10       | 0.38          |
| (1,3079) | 1:93:A:THR:HG23  | 1:41:A:THR:H     | 9        | 0.38          |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H     | 12       | 0.38          |
| (1,3052) | 1:29:A:LEU:HD13  | 1:42:A:GLN:H     | 7        | 0.38          |
| (1,2979) | 1:110:A:SER:H    | 1:80:A:ILE:HG12  | 12       | 0.38          |
| (1,2868) | 1:12:A:VAL:H     | 1:12:A:VAL:HB    | 19       | 0.38          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG23 | 11       | 0.38          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG23 | 19       | 0.38          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD12  | 4        | 0.38          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 4        | 0.38          |
| (1,2649) | 1:100:A:GLY:H    | 1:98:A:ALA:HB1   | 16       | 0.38          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG22  | 16       | 0.38          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 3        | 0.38          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG11  | 17       | 0.38          |
| (1,2567) | 1:113:A:LYS:H    | 1:114:A:ALA:HB3  | 4        | 0.38          |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG23  | 20       | 0.38          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG21  | 10       | 0.38          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD12 | 11       | 0.38          |
| (1,2381) | 1:104:A:VAL:HG11 | 1:19:A:LEU:HG    | 12       | 0.38          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:105:A:THR:HB   | 14       | 0.38          |
| (1,2358) | 1:45:A:THR:HA    | 1:90:A:ILE:HD12  | 8        | 0.38          |
| (1,2278) | 1:140:A:LYS:HB3  | 1:137:A:GLU:HG2  | 15       | 0.38          |
| (1,2169) | 1:56:A:ILE:HG23  | 1:58:A:VAL:HB    | 7        | 0.38          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG2   | 3        | 0.37          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG23 | 13       | 0.37          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG23 | 19       | 0.37          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG22 | 20       | 0.37          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG23 | 17       | 0.37          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG21  | 1        | 0.37          |
| (1,2717) | 1:19:A:LEU:H     | 1:29:A:LEU:HD11  | 19       | 0.37          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD23 | 3        | 0.37          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD13 | 8        | 0.37          |
| (1,2412) | 1:102:A:LEU:H    | 1:118:A:THR:HG22 | 11       | 0.37          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG23 | 1        | 0.37          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG22  | 13       | 0.37          |
| (1,2380) | 1:104:A:VAL:HG11 | 1:105:A:THR:HB   | 16       | 0.37          |
| (1,2181) | 1:138:A:ALA:HB3  | 1:134:A:MET:HB3  | 3        | 0.37          |
| (1,3183) | 1:12:A:VAL:HG23  | 1:35:A:THR:HA    | 17       | 0.36          |
| (1,3161) | 1:36:A:ILE:HD12  | 1:11:A:ASP:H     | 3        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3128) | 1:141:A:TYR:HD1  | 1:144:A:GLU:HG2  | 16       | 0.36          |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H     | 2        | 0.36          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 11       | 0.36          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG23 | 2        | 0.36          |
| (1,2750) | 1:11:A:ASP:H     | 1:12:A:VAL:HG11  | 7        | 0.36          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG2  | 6        | 0.36          |
| (1,2698) | 1:127:A:SER:H    | 1:130:A:GLU:HG3  | 15       | 0.36          |
| (1,2593) | 1:64:A:ALA:H     | 1:66:A:THR:HA    | 19       | 0.36          |
| (1,2570) | 1:80:A:ILE:H     | 1:54:A:VAL:HG23  | 3        | 0.36          |
| (1,2530) | 1:90:A:ILE:H     | 1:43:A:ILE:HG21  | 14       | 0.36          |
| (1,2495) | 1:57:A:GLN:H     | 1:74:A:ARG:HB2   | 20       | 0.36          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD12 | 19       | 0.36          |
| (1,2411) | 1:102:A:LEU:H    | 1:96:A:ILE:HD11  | 4        | 0.36          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG22  | 16       | 0.36          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG22  | 20       | 0.36          |
| (1,2379) | 1:158:A:LEU:HD11 | 1:44:A:PHE:H     | 11       | 0.36          |
| (1,2344) | 1:256:A:VAL:HA   | 1:255:A:GLU:HG3  | 8        | 0.36          |
| (1,2278) | 1:133:A:ARG:HG3  | 1:137:A:GLU:HG2  | 6        | 0.36          |
| (1,2228) | 1:88:A:PRO:HG2   | 1:88:A:PRO:HA    | 14       | 0.36          |
| (1,2169) | 1:56:A:ILE:HG22  | 1:58:A:VAL:HB    | 9        | 0.36          |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 19       | 0.36          |
| (1,2039) | 1:74:A:ARG:HA    | 1:55:A:LEU:HD12  | 2        | 0.36          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 11       | 0.35          |
| (1,3160) | 1:143:A:ALA:HA   | 1:142:A:LYS:HB3  | 5        | 0.35          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 12       | 0.35          |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD12 | 19       | 0.35          |
| (1,2931) | 1:62:A:GLU:H     | 1:62:A:GLU:HG3   | 7        | 0.35          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG22 | 9        | 0.35          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 10       | 0.35          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG22 | 20       | 0.35          |
| (1,2824) | 1:146:A:GLU:H    | 1:143:A:ALA:HA   | 9        | 0.35          |
| (1,2790) | 1:15:A:LEU:H     | 1:14:A:PRO:HG2   | 13       | 0.35          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG21  | 4        | 0.35          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG22  | 2        | 0.35          |
| (1,2582) | 1:51:A:GLN:H     | 1:48:A:SER:HB2   | 5        | 0.35          |
| (1,2567) | 1:113:A:LYS:H    | 1:111:A:THR:HG22 | 2        | 0.35          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 9        | 0.35          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 14       | 0.35          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG23  | 2        | 0.35          |
| (1,2548) | 1:95:A:ASP:H     | 1:30:A:ILE:HD13  | 3        | 0.35          |
| (1,2548) | 1:95:A:ASP:H     | 1:30:A:ILE:HD11  | 16       | 0.35          |
| (1,2516) | 1:96:A:ILE:H     | 1:39:A:LYS:HB2   | 11       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2495) | 1:57:A:GLN:H     | 1:74:A:ARG:HB3   | 19       | 0.35          |
| (1,2387) | 1:29:A:LEU:HD11  | 1:92:A:VAL:HG13  | 7        | 0.35          |
| (1,2222) | 1:158:A:LEU:HD21 | 1:19:A:LEU:HD11  | 1        | 0.35          |
| (1,2122) | 1:29:A:LEU:HD21  | 1:93:A:THR:HA    | 1        | 0.35          |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 14       | 0.35          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 20       | 0.34          |
| (1,3151) | 1:13:A:ALA:HA    | 1:96:A:ILE:HG23  | 16       | 0.34          |
| (1,3149) | 1:13:A:ALA:HB3   | 1:14:A:PRO:HD2   | 7        | 0.34          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB3   | 15       | 0.34          |
| (1,2980) | 1:111:A:THR:H    | 1:81:A:PRO:HG3   | 5        | 0.34          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB2   | 1        | 0.34          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG21 | 17       | 0.34          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 12       | 0.34          |
| (1,2824) | 1:146:A:GLU:H    | 1:143:A:ALA:HA   | 14       | 0.34          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG3  | 10       | 0.34          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB1   | 4        | 0.34          |
| (1,2699) | 1:127:A:SER:H    | 1:126:A:LEU:HD21 | 15       | 0.34          |
| (1,2698) | 1:127:A:SER:H    | 1:130:A:GLU:HB2  | 17       | 0.34          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD12  | 10       | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 1        | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 3        | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD12 | 5        | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD12 | 11       | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 13       | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 15       | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 18       | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD12 | 19       | 0.34          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 20       | 0.34          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG23  | 17       | 0.34          |
| (1,2531) | 1:90:A:ILE:H     | 1:90:A:ILE:HG13  | 6        | 0.34          |
| (1,2501) | 1:31:A:LYS:H     | 1:28:A:ALA:HB2   | 8        | 0.34          |
| (1,2412) | 1:102:A:LEU:H    | 1:118:A:THR:HG23 | 14       | 0.34          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG23  | 5        | 0.34          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG23  | 14       | 0.34          |
| (1,2380) | 1:104:A:VAL:HG12 | 1:93:A:THR:HB    | 7        | 0.34          |
| (1,2199) | 1:117:A:ILE:HD13 | 1:75:A:PHE:H     | 17       | 0.34          |
| (1,2075) | 1:130:A:GLU:H    | 1:130:A:GLU:HG3  | 18       | 0.34          |
| (1,2074) | 1:11:A:ASP:HB3   | 1:36:A:ILE:HG12  | 12       | 0.34          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG21  | 12       | 0.33          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG23  | 13       | 0.33          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 7        | 0.33          |
| (1,3173) | 1:70:A:ASN:HD22  | 1:126:A:LEU:HB2  | 2        | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB1   | 14       | 0.33          |
| (1,3117) | 1:126:A:LEU:HB2  | 1:70:A:ASN:HD22  | 2        | 0.33          |
| (1,2980) | 1:111:A:THR:H    | 1:81:A:PRO:HG3   | 4        | 0.33          |
| (1,2904) | 1:18:A:GLY:H     | 1:19:A:LEU:HD21  | 19       | 0.33          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG23 | 18       | 0.33          |
| (1,2851) | 1:126:A:LEU:H    | 1:126:A:LEU:HD22 | 9        | 0.33          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 1        | 0.33          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 3        | 0.33          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 6        | 0.33          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 7        | 0.33          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG22 | 8        | 0.33          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 13       | 0.33          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG23 | 14       | 0.33          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG23  | 2        | 0.33          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG23  | 8        | 0.33          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG22  | 13       | 0.33          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB3   | 7        | 0.33          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG22  | 15       | 0.33          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD11 | 2        | 0.33          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD12 | 4        | 0.33          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD13 | 7        | 0.33          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD13 | 10       | 0.33          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD13 | 16       | 0.33          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD12 | 17       | 0.33          |
| (1,2548) | 1:95:A:ASP:H     | 1:30:A:ILE:HD12  | 10       | 0.33          |
| (1,2516) | 1:96:A:ILE:H     | 1:39:A:LYS:HB2   | 15       | 0.33          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG23  | 2        | 0.33          |
| (1,2381) | 1:104:A:VAL:HG13 | 1:19:A:LEU:HG    | 2        | 0.33          |
| (1,2381) | 1:104:A:VAL:HG13 | 1:19:A:LEU:HG    | 4        | 0.33          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD12  | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD12  | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD12  | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD12  | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD12  | 1:17:A:LEU:HB2   | 18       | 0.33          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3   | 18       | 0.33          |
| (1,2228) | 1:88:A:PRO:HG2  | 1:88:A:PRO:HA    | 6        | 0.33          |
| (1,3180) | 1:35:A:THR:HA   | 1:36:A:ILE:HG12  | 1        | 0.32          |
| (1,3157) | 1:24:A:GLY:H    | 1:159:A:GLU:HG3  | 9        | 0.32          |
| (1,3141) | 1:13:A:ALA:HB1  | 1:32:A:ARG:HB2   | 18       | 0.32          |
| (1,3133) | 1:75:A:PHE:HD2  | 1:117:A:ILE:HD13 | 18       | 0.32          |
| (1,3006) | 1:145:A:ASP:H   | 1:144:A:GLU:HB2  | 16       | 0.32          |
| (1,2950) | 1:69:A:ASN:H    | 1:67:A:LYS:HG3   | 10       | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB2   | 11       | 0.32          |
| (1,2933) | 1:63:A:ARG:H     | 1:62:A:GLU:HG2   | 2        | 0.32          |
| (1,2918) | 1:45:A:THR:H     | 1:158:A:LEU:HG   | 7        | 0.32          |
| (1,2868) | 1:12:A:VAL:H     | 1:12:A:VAL:HB    | 17       | 0.32          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG23 | 4        | 0.32          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG22 | 16       | 0.32          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 18       | 0.32          |
| (1,2844) | 1:118:A:THR:H    | 1:117:A:ILE:HB   | 10       | 0.32          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD23  | 9        | 0.32          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG2  | 2        | 0.32          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG23  | 10       | 0.32          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB2   | 5        | 0.32          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG22  | 13       | 0.32          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD12  | 4        | 0.32          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 11       | 0.32          |
| (1,2582) | 1:51:A:GLN:H     | 1:48:A:SER:HB2   | 16       | 0.32          |
| (1,2561) | 1:101:A:ILE:H    | 1:101:A:ILE:HD13 | 8        | 0.32          |
| (1,2550) | 1:95:A:ASP:H     | 1:102:A:LEU:HB2  | 20       | 0.32          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG2  | 8        | 0.32          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG23  | 6        | 0.32          |
| (1,2530) | 1:90:A:ILE:H     | 1:43:A:ILE:HG21  | 19       | 0.32          |
| (1,2527) | 1:104:A:VAL:H    | 1:75:A:PHE:HE1   | 4        | 0.32          |
| (1,2420) | 1:119:A:ILE:H    | 1:101:A:ILE:HG23 | 16       | 0.32          |
| (1,2381) | 1:104:A:VAL:HG12 | 1:19:A:LEU:HG    | 3        | 0.32          |
| (1,2368) | 1:115:A:ASN:HA   | 1:75:A:PHE:HE1   | 20       | 0.32          |
| (1,2344) | 1:253:A:ILE:HA   | 1:254:A:GLU:HG2  | 14       | 0.32          |
| (1,2274) | 1:116:A:LYS:HA   | 1:116:A:LYS:HE2  | 19       | 0.32          |
| (1,2169) | 1:56:A:ILE:HG21  | 1:58:A:VAL:HB    | 10       | 0.32          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22  | 17       | 0.31          |
| (1,3189) | 1:12:A:VAL:HG12  | 1:33:A:ASN:HA    | 4        | 0.31          |
| (1,3174) | 1:70:A:ASN:HD21  | 1:15:A:LEU:HB2   | 14       | 0.31          |
| (1,3173) | 1:70:A:ASN:HD22  | 1:126:A:LEU:HB2  | 1        | 0.31          |
| (1,3159) | 1:15:A:LEU:HD22  | 1:136:A:GLN:H    | 9        | 0.31          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB3   | 9        | 0.31          |
| (1,3117) | 1:126:A:LEU:HB2  | 1:70:A:ASN:HD22  | 1        | 0.31          |
| (1,3117) | 1:15:A:LEU:HB2   | 1:70:A:ASN:HD21  | 14       | 0.31          |
| (1,3073) | 1:77:A:LEU:HD13  | 1:115:A:ASN:H    | 17       | 0.31          |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H     | 16       | 0.31          |
| (1,3052) | 1:29:A:LEU:HD22  | 1:42:A:GLN:H     | 3        | 0.31          |
| (1,3031) | 1:131:A:ILE:H    | 1:126:A:LEU:HD22 | 13       | 0.31          |
| (1,2969) | 1:100:A:GLY:H    | 1:101:A:ILE:HD12 | 17       | 0.31          |
| (1,2931) | 1:62:A:GLU:H     | 1:62:A:GLU:HG3   | 1        | 0.31          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2844) | 1:118:A:THR:H   | 1:116:A:LYS:HD2  | 15       | 0.31          |
| (1,2790) | 1:15:A:LEU:H    | 1:14:A:PRO:HG2   | 3        | 0.31          |
| (1,2743) | 1:135:A:VAL:H   | 1:134:A:MET:HG2  | 7        | 0.31          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB3   | 10       | 0.31          |
| (1,2567) | 1:113:A:LYS:H   | 1:114:A:ALA:HB2  | 15       | 0.31          |
| (1,2556) | 1:40:A:GLN:H    | 1:93:A:THR:HG21  | 4        | 0.31          |
| (1,2332) | 1:17:A:LEU:H    | 1:13:A:ALA:HB1   | 19       | 0.31          |
| (1,2211) | 1:58:A:VAL:HG22 | 1:73:A:GLY:H     | 16       | 0.31          |
| (1,1963) | 1:80:A:ILE:HD12 | 1:77:A:LEU:HA    | 10       | 0.31          |
| (1,3197) | 1:132:A:GLU:HB3 | 1:15:A:LEU:HD23  | 7        | 0.3           |
| (1,3192) | 1:13:A:ALA:H    | 1:12:A:VAL:HG21  | 19       | 0.3           |
| (1,3180) | 1:35:A:THR:HA   | 1:36:A:ILE:HG12  | 16       | 0.3           |
| (1,3155) | 1:14:A:PRO:HA   | 1:13:A:ALA:HB3   | 15       | 0.3           |
| (1,3125) | 1:75:A:PHE:HD2  | 1:117:A:ILE:HG22 | 13       | 0.3           |
| (1,3053) | 1:149:A:ARG:HB2 | 1:26:A:MET:H     | 17       | 0.3           |
| (1,3011) | 1:157:A:ALA:H   | 1:158:A:LEU:HG   | 18       | 0.3           |
| (1,3006) | 1:145:A:ASP:H   | 1:144:A:GLU:HB2  | 5        | 0.3           |
| (1,2918) | 1:45:A:THR:H    | 1:158:A:LEU:HG   | 10       | 0.3           |
| (1,2868) | 1:12:A:VAL:H    | 1:12:A:VAL:HB    | 1        | 0.3           |
| (1,2790) | 1:15:A:LEU:H    | 1:14:A:PRO:HG2   | 5        | 0.3           |
| (1,2750) | 1:11:A:ASP:H    | 1:12:A:VAL:HG13  | 6        | 0.3           |
| (1,2743) | 1:135:A:VAL:H   | 1:134:A:MET:HG3  | 3        | 0.3           |
| (1,2725) | 1:38:A:THR:H    | 1:38:A:THR:HG21  | 11       | 0.3           |
| (1,2725) | 1:38:A:THR:H    | 1:38:A:THR:HG22  | 17       | 0.3           |
| (1,2582) | 1:51:A:GLN:H    | 1:48:A:SER:HB2   | 4        | 0.3           |
| (1,2544) | 1:114:A:ALA:H   | 1:113:A:LYS:HB3  | 10       | 0.3           |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG2  | 16       | 0.3           |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG22  | 8        | 0.3           |
| (1,2530) | 1:90:A:ILE:H    | 1:43:A:ILE:HG22  | 13       | 0.3           |
| (1,2411) | 1:102:A:LEU:H   | 1:96:A:ILE:HD12  | 1        | 0.3           |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD13  | 4        | 0.3           |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD11  | 5        | 0.3           |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD11  | 8        | 0.3           |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD12  | 14       | 0.3           |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD11  | 17       | 0.3           |
| (1,2216) | 1:13:A:ALA:HB2  | 1:32:A:ARG:HB3   | 20       | 0.3           |
| (1,2182) | 1:54:A:VAL:HG23 | 1:76:A:GLU:HA    | 12       | 0.3           |
| (1,1963) | 1:80:A:ILE:HD13 | 1:77:A:LEU:HA    | 6        | 0.3           |
| (1,3192) | 1:13:A:ALA:H    | 1:12:A:VAL:HG22  | 5        | 0.29          |
| (1,3173) | 1:70:A:ASN:HD22 | 1:15:A:LEU:HB2   | 3        | 0.29          |
| (1,3159) | 1:15:A:LEU:HD21 | 1:131:A:ILE:H    | 16       | 0.29          |
| (1,3145) | 1:87:A:VAL:HA   | 1:83:A:ALA:HB3   | 12       | 0.29          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3065) | 1:92:A:VAL:HG13 | 1:93:A:THR:H     | 20       | 0.29          |
| (1,2996) | 1:146:A:GLU:H   | 1:142:A:LYS:HG3  | 8        | 0.29          |
| (1,2868) | 1:12:A:VAL:H    | 1:12:A:VAL:HB    | 10       | 0.29          |
| (1,2846) | 1:118:A:THR:H   | 1:117:A:ILE:HG22 | 5        | 0.29          |
| (1,2833) | 1:116:A:LYS:H   | 1:75:A:PHE:HE2   | 1        | 0.29          |
| (1,2833) | 1:116:A:LYS:H   | 1:75:A:PHE:HE2   | 10       | 0.29          |
| (1,2824) | 1:146:A:GLU:H   | 1:143:A:ALA:HA   | 19       | 0.29          |
| (1,2820) | 1:136:A:GLN:H   | 1:135:A:VAL:HG13 | 12       | 0.29          |
| (1,2716) | 1:19:A:LEU:H    | 1:28:A:ALA:HB1   | 12       | 0.29          |
| (1,2699) | 1:127:A:SER:H   | 1:126:A:LEU:HD21 | 2        | 0.29          |
| (1,2642) | 1:46:A:THR:H    | 1:45:A:THR:HG21  | 10       | 0.29          |
| (1,2567) | 1:113:A:LYS:H   | 1:111:A:THR:HG21 | 7        | 0.29          |
| (1,2556) | 1:40:A:GLN:H    | 1:93:A:THR:HG21  | 7        | 0.29          |
| (1,2549) | 1:95:A:ASP:H    | 1:93:A:THR:HG23  | 12       | 0.29          |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG2  | 14       | 0.29          |
| (1,2404) | 1:92:A:VAL:H    | 1:41:A:THR:HG21  | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2   | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2   | 18       | 0.29          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 18       | 0.29          |
| (1,2256) | 1:94:A:PHE:HE2  | 1:19:A:LEU:HB2 | 15       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 8        | 0.29          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 8        | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 17       | 0.29          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 17       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 16       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 16       | 0.29          |
| (1,2223) | 1:90:A:ILE:HB   | 1:90:A:ILE:HD12 | 1        | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD12  | 9        | 0.29          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD13  | 11       | 0.29          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD13  | 12       | 0.29          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD11  | 15       | 0.29          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD12  | 16       | 0.29          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD12  | 18       | 0.29          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD11  | 20       | 0.29          |
| (1,2186) | 1:96:A:ILE:HG21  | 1:36:A:ILE:HD13  | 14       | 0.29          |
| (1,2169) | 1:56:A:ILE:HG21  | 1:58:A:VAL:HB    | 13       | 0.29          |
| (1,1966) | 1:119:A:ILE:HD11 | 1:119:A:ILE:HB   | 15       | 0.29          |
| (1,1963) | 1:80:A:ILE:HD12  | 1:52:A:PRO:HA    | 17       | 0.29          |
| (1,3189) | 1:12:A:VAL:HG11  | 1:33:A:ASN:HA    | 5        | 0.28          |
| (1,3189) | 1:12:A:VAL:HG13  | 1:33:A:ASN:HA    | 19       | 0.28          |
| (1,3157) | 1:24:A:GLY:H     | 1:159:A:GLU:HG3  | 16       | 0.28          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB2   | 2        | 0.28          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB3   | 10       | 0.28          |
| (1,3142) | 1:131:A:ILE:HD13 | 1:131:A:ILE:HB   | 2        | 0.28          |
| (1,3125) | 1:75:A:PHE:HD2   | 1:117:A:ILE:HG21 | 19       | 0.28          |
| (1,3073) | 1:77:A:LEU:HD11  | 1:115:A:ASN:H    | 8        | 0.28          |
| (1,2960) | 1:86:A:GLY:H     | 1:87:A:VAL:HG22  | 15       | 0.28          |
| (1,2895) | 1:43:A:ILE:H     | 1:43:A:ILE:HG13  | 18       | 0.28          |
| (1,2868) | 1:12:A:VAL:H     | 1:12:A:VAL:HB    | 9        | 0.28          |
| (1,2868) | 1:12:A:VAL:H     | 1:10:A:LEU:HB2   | 18       | 0.28          |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HE2   | 2        | 0.28          |
| (1,2790) | 1:15:A:LEU:H     | 1:14:A:PRO:HG2   | 8        | 0.28          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD22  | 20       | 0.28          |
| (1,2748) | 1:11:A:ASP:H     | 1:36:A:ILE:HG12  | 2        | 0.28          |
| (1,2717) | 1:19:A:LEU:H     | 1:29:A:LEU:HD12  | 10       | 0.28          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB1   | 3        | 0.28          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB2   | 6        | 0.28          |
| (1,2716) | 1:19:A:LEU:H     | 1:29:A:LEU:HB2   | 17       | 0.28          |
| (1,2698) | 1:127:A:SER:H    | 1:130:A:GLU:HB2  | 18       | 0.28          |
| (1,2689) | 1:45:A:THR:H     | 1:158:A:LEU:HD11 | 18       | 0.28          |
| (1,2649) | 1:100:A:GLY:H    | 1:98:A:ALA:HB3   | 11       | 0.28          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG21  | 7        | 0.28          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD12  | 9        | 0.28          |
| (1,2567) | 1:113:A:LYS:H    | 1:111:A:THR:HG21 | 6        | 0.28          |
| (1,2567) | 1:113:A:LYS:H    | 1:111:A:THR:HG21 | 10       | 0.28          |
| (1,2507) | 1:104:A:VAL:H    | 1:117:A:ILE:HB   | 17       | 0.28          |
| (1,2344) | 1:253:A:ILE:HA   | 1:254:A:GLU:HG3  | 4        | 0.28          |
| (1,2344) | 1:256:A:VAL:HA   | 1:255:A:GLU:HG2  | 19       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11  | 1:17:A:LEU:HB2   | 2        | 0.28          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 2        | 0.28          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 2        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 5        | 0.28          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 5        | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 16       | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD21  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB2   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB2   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB2   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB2   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB2   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB2   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB2   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB2   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB3   | 16       | 0.28          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD13  | 2        | 0.28          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD11  | 3        | 0.28          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD11  | 10       | 0.28          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD12  | 13       | 0.28          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD11  | 19       | 0.28          |
| (1,2220) | 1:143:A:ALA:HB1  | 1:146:A:GLU:HB2  | 2        | 0.28          |
| (1,2188) | 1:80:A:ILE:HG23  | 1:53:A:GLY:HA2   | 16       | 0.28          |
| (1,1966) | 1:119:A:ILE:HD12 | 1:119:A:ILE:HB   | 3        | 0.28          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG23  | 2        | 0.27          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG21  | 10       | 0.27          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 6        | 0.27          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 6        | 0.27          |
| (1,3165) | 1:96:A:ILE:HG22  | 1:38:A:THR:H     | 7        | 0.27          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB1   | 3        | 0.27          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB1   | 13       | 0.27          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB2   | 16       | 0.27          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 12       | 0.27          |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H     | 13       | 0.27          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 7        | 0.27          |
| (1,2946) | 1:68:A:ASP:H     | 1:69:A:ASN:HA    | 8        | 0.27          |
| (1,2946) | 1:68:A:ASP:H     | 1:69:A:ASN:HA    | 20       | 0.27          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG21 | 9        | 0.27          |
| (1,2884) | 1:133:A:ARG:H    | 1:133:A:ARG:HG3  | 6        | 0.27          |
| (1,2868) | 1:12:A:VAL:H     | 1:12:A:VAL:HB    | 11       | 0.27          |
| (1,2846) | 1:118:A:THR:H    | 1:117:A:ILE:HG21 | 15       | 0.27          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2833) | 1:116:A:LYS:H   | 1:75:A:PHE:HE1   | 19       | 0.27          |
| (1,2712) | 1:137:A:GLU:H   | 1:138:A:ALA:HB1  | 20       | 0.27          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB2   | 2        | 0.27          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB1   | 6        | 0.27          |
| (1,2642) | 1:46:A:THR:H    | 1:45:A:THR:HG21  | 6        | 0.27          |
| (1,2604) | 1:43:A:ILE:H    | 1:43:A:ILE:HD11  | 14       | 0.27          |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG22  | 3        | 0.27          |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG23  | 12       | 0.27          |
| (1,2526) | 1:42:A:GLN:H    | 1:94:A:PHE:H     | 16       | 0.27          |
| (1,2463) | 1:108:A:ASP:H   | 1:77:A:LEU:HG    | 18       | 0.27          |
| (1,2447) | 1:97:A:ASP:H    | 1:101:A:ILE:HD11 | 13       | 0.27          |
| (1,2447) | 1:97:A:ASP:H    | 1:101:A:ILE:HD11 | 14       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 18       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3  | 18       | 0.27          |
| (1,2278) | 1:140:A:LYS:HB3 | 1:137:A:GLU:HG2 | 11       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2  | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3  | 12       | 0.27          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 12       | 0.27          |
| (1,2256) | 1:94:A:PHE:HE2  | 1:19:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 3        | 0.27          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 3        | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 10       | 0.27          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 10       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 20       | 0.27          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 20       | 0.27          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 20       | 0.27          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3 | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3 | 3        | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2   | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2   | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2   | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2   | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 3        | 0.27          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 3        | 0.27          |
| (1,2178) | 1:26:A:MET:HE2   | 1:69:A:ASN:HB3   | 1        | 0.27          |
| (1,2075) | 1:130:A:GLU:H    | 1:129:A:GLU:HG3  | 3        | 0.27          |
| (1,1966) | 1:119:A:ILE:HD13 | 1:119:A:ILE:HB   | 8        | 0.27          |
| (1,1966) | 1:119:A:ILE:HD11 | 1:119:A:ILE:HB   | 14       | 0.27          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG23  | 7        | 0.26          |
| (1,3189) | 1:12:A:VAL:HG13  | 1:33:A:ASN:HA    | 9        | 0.26          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 17       | 0.26          |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 8        | 0.26          |
| (1,3175) | 1:157:A:ALA:HB1  | 1:44:A:PHE:HB3   | 19       | 0.26          |
| (1,3173) | 1:70:A:ASN:HD22  | 1:126:A:LEU:HB3  | 4        | 0.26          |
| (1,3135) | 1:83:A:ALA:H     | 1:82:A:PRO:HB2   | 14       | 0.26          |
| (1,3122) | 1:101:A:ILE:HG23 | 1:103:A:ASN:HD21 | 14       | 0.26          |
| (1,3117) | 1:126:A:LEU:HB3  | 1:70:A:ASN:HD22  | 4        | 0.26          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 13       | 0.26          |
| (1,3065) | 1:92:A:VAL:HG13  | 1:93:A:THR:H     | 6        | 0.26          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 20       | 0.26          |
| (1,2940) | 1:67:A:LYS:H     | 1:68:A:ASP:HB2   | 2        | 0.26          |
| (1,2931) | 1:62:A:GLU:H     | 1:62:A:GLU:HG3   | 8        | 0.26          |
| (1,2909) | 1:147:A:VAL:H    | 1:146:A:GLU:HB2  | 9        | 0.26          |
| (1,2873) | 1:103:A:ASN:HD21 | 1:101:A:ILE:HG23 | 14       | 0.26          |
| (1,2868) | 1:12:A:VAL:H     | 1:10:A:LEU:HB3   | 16       | 0.26          |
| (1,2844) | 1:118:A:THR:H    | 1:117:A:ILE:HB   | 11       | 0.26          |
| (1,2790) | 1:15:A:LEU:H     | 1:14:A:PRO:HG2   | 17       | 0.26          |
| (1,2761) | 1:30:A:ILE:H     | 1:30:A:ILE:HD12  | 19       | 0.26          |
| (1,2750) | 1:11:A:ASP:H     | 1:12:A:VAL:HG13  | 11       | 0.26          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG21  | 3        | 0.26          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG23  | 12       | 0.26          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG21  | 14       | 0.26          |
| (1,2717) | 1:19:A:LEU:H     | 1:29:A:LEU:HD13  | 4        | 0.26          |
| (1,2717) | 1:19:A:LEU:H     | 1:29:A:LEU:HD13  | 6        | 0.26          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB1   | 14       | 0.26          |
| (1,2698) | 1:127:A:SER:H    | 1:130:A:GLU:HB2  | 19       | 0.26          |
| (1,2684) | 1:158:A:LEU:H    | 1:90:A:ILE:HG13  | 20       | 0.26          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG21  | 11       | 0.26          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2582) | 1:51:A:GLN:H    | 1:48:A:SER:HB2   | 13       | 0.26          |
| (1,2530) | 1:90:A:ILE:H    | 1:43:A:ILE:HG23  | 12       | 0.26          |
| (1,2412) | 1:102:A:LEU:H   | 1:118:A:THR:HG22 | 13       | 0.26          |
| (1,2344) | 1:256:A:VAL:HA  | 1:255:A:GLU:HG2  | 10       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 11       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 11       | 0.26          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 3        | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 3        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 6        | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 6        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 7        | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 7        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 9        | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 9        | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 11       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 11       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 14       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 14       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 14       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 15       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 15       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 16       | 0.26          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 16       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 20       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD21  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD21  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD22  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23  | 1:55:A:LEU:HB2   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2266) | 1:55:A:LEU:HD23  | 1:55:A:LEU:HB3   | 20       | 0.26          |
| (1,2223) | 1:90:A:ILE:HB    | 1:90:A:ILE:HD13  | 7        | 0.26          |
| (1,2175) | 1:26:A:MET:HE1   | 1:58:A:VAL:HA    | 7        | 0.26          |
| (1,2169) | 1:56:A:ILE:HG22  | 1:74:A:ARG:HB2   | 2        | 0.26          |
| (1,2144) | 1:27:A:THR:HG22  | 1:156:A:ASN:HD22 | 2        | 0.26          |
| (1,1966) | 1:119:A:ILE:HD11 | 1:119:A:ILE:HB   | 6        | 0.26          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG23  | 1        | 0.25          |
| (1,3157) | 1:24:A:GLY:H     | 1:159:A:GLU:HG3  | 11       | 0.25          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB2   | 5        | 0.25          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB1   | 1        | 0.25          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 7        | 0.25          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 4        | 0.25          |
| (1,3073) | 1:77:A:LEU:HD12  | 1:115:A:ASN:H    | 15       | 0.25          |
| (1,3065) | 1:92:A:VAL:HG12  | 1:93:A:THR:H     | 4        | 0.25          |
| (1,3008) | 1:148:A:GLN:H    | 1:151:A:ARG:HB2  | 13       | 0.25          |
| (1,2881) | 1:17:A:LEU:H     | 1:15:A:LEU:HB3   | 3        | 0.25          |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HE1   | 9        | 0.25          |
| (1,2790) | 1:15:A:LEU:H     | 1:14:A:PRO:HG2   | 7        | 0.25          |
| (1,2750) | 1:11:A:ASP:H     | 1:12:A:VAL:HG22  | 10       | 0.25          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 16       | 0.25          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD11  | 19       | 0.25          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2568) | 1:113:A:LYS:H   | 1:113:A:LYS:HG3  | 2        | 0.25          |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG2  | 6        | 0.25          |
| (1,2420) | 1:119:A:ILE:H   | 1:101:A:ILE:HG23 | 10       | 0.25          |
| (1,2358) | 1:45:A:THR:HA   | 1:158:A:LEU:HD13 | 7        | 0.25          |
| (1,2344) | 1:256:A:VAL:HA  | 1:255:A:GLU:HG2  | 1        | 0.25          |
| (1,2344) | 1:253:A:ILE:HA  | 1:254:A:GLU:HG3  | 6        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3   | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3   | 1        | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 1        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 2        | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 2        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 4        | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 4        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 5        | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 5        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 8        | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 8        | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 10       | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 10       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 10       | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 13       | 0.25          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 13       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 19       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB2   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB2   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB3   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD22  | 1:17:A:LEU:HB3   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB2   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB2   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB3   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB3   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB2   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB2   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB3   | 19       | 0.25          |
| (1,2254) | 1:17:A:LEU:HD23  | 1:17:A:LEU:HB3   | 19       | 0.25          |
| (1,2181) | 1:138:A:ALA:HB1  | 1:134:A:MET:HB3  | 4        | 0.25          |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 12       | 0.25          |
| (1,2074) | 1:11:A:ASP:HB3   | 1:36:A:ILE:HG12  | 5        | 0.25          |
| (1,1963) | 1:80:A:ILE:HD12  | 1:52:A:PRO:HA    | 5        | 0.25          |
| (1,394)  | 1:75:A:PHE:HD1   | 1:74:A:ARG:HA    | 17       | 0.25          |
| (1,394)  | 1:75:A:PHE:HD2   | 1:74:A:ARG:HA    | 17       | 0.25          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG21  | 14       | 0.24          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22  | 16       | 0.24          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 3        | 0.24          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 5        | 0.24          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 19       | 0.24          |
| (1,3149) | 1:13:A:ALA:HB2   | 1:14:A:PRO:HD2   | 5        | 0.24          |
| (1,3128) | 1:141:A:TYR:HD1  | 1:137:A:GLU:HG2  | 12       | 0.24          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 5        | 0.24          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 11       | 0.24          |
| (1,3053) | 1:149:A:ARG:HB2  | 1:26:A:MET:H     | 12       | 0.24          |
| (1,3052) | 1:29:A:LEU:HD11  | 1:42:A:GLN:H     | 2        | 0.24          |
| (1,3033) | 1:103:A:ASN:HD21 | 1:117:A:ILE:HG13 | 19       | 0.24          |
| (1,3011) | 1:157:A:ALA:H    | 1:158:A:LEU:HG   | 8        | 0.24          |
| (1,3008) | 1:148:A:GLN:H    | 1:151:A:ARG:HB2  | 4        | 0.24          |
| (1,2809) | 1:132:A:GLU:H    | 1:131:A:ILE:HG22 | 14       | 0.24          |
| (1,2698) | 1:127:A:SER:H    | 1:131:A:ILE:HG13 | 11       | 0.24          |
| (1,2604) | 1:43:A:ILE:H     | 1:43:A:ILE:HD12  | 2        | 0.24          |
| (1,2549) | 1:95:A:ASP:H     | 1:93:A:THR:HG21  | 13       | 0.24          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG3  | 2        | 0.24          |
| (1,2526) | 1:42:A:GLN:H     | 1:94:A:PHE:H     | 20       | 0.24          |
| (1,2430) | 1:27:A:THR:H     | 1:29:A:LEU:HD13  | 4        | 0.24          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG22  | 12       | 0.24          |
| (1,2392) | 1:36:A:ILE:HD13  | 1:14:A:PRO:HD3   | 3        | 0.24          |
| (1,2387) | 1:29:A:LEU:HD23  | 1:92:A:VAL:HG11  | 3        | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2387) | 1:29:A:LEU:HD22  | 1:92:A:VAL:HG12  | 12       | 0.24          |
| (1,2381) | 1:104:A:VAL:HG13 | 1:19:A:LEU:HG    | 14       | 0.24          |
| (1,2169) | 1:56:A:ILE:HG21  | 1:58:A:VAL:HB    | 3        | 0.24          |
| (1,2122) | 1:29:A:LEU:HD21  | 1:93:A:THR:HA    | 13       | 0.24          |
| (1,1982) | 1:252:A:THR:HA   | 1:252:A:THR:HG21 | 15       | 0.24          |
| (1,1933) | 1:64:A:ALA:HB1   | 1:145:A:ASP:HB2  | 15       | 0.24          |
| (1,1933) | 1:64:A:ALA:HB2   | 1:145:A:ASP:HB2  | 15       | 0.24          |
| (1,1933) | 1:64:A:ALA:HB3   | 1:145:A:ASP:HB2  | 15       | 0.24          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22  | 3        | 0.23          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22  | 11       | 0.23          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 18       | 0.23          |
| (1,3159) | 1:15:A:LEU:HD12  | 1:131:A:ILE:H    | 5        | 0.23          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB1   | 12       | 0.23          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB1   | 3        | 0.23          |
| (1,3128) | 1:141:A:TYR:HD2  | 1:144:A:GLU:HG3  | 2        | 0.23          |
| (1,3118) | 1:131:A:ILE:HD12 | 1:70:A:ASN:HD22  | 18       | 0.23          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 9        | 0.23          |
| (1,3073) | 1:77:A:LEU:HD13  | 1:115:A:ASN:H    | 6        | 0.23          |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H     | 10       | 0.23          |
| (1,3056) | 1:74:A:ARG:HB3   | 1:58:A:VAL:H     | 15       | 0.23          |
| (1,3052) | 1:29:A:LEU:HD11  | 1:42:A:GLN:H     | 18       | 0.23          |
| (1,3045) | 1:33:A:ASN:HA    | 1:13:A:ALA:H     | 2        | 0.23          |
| (1,3028) | 1:59:A:TYR:H     | 1:60:A:GLU:HG3   | 1        | 0.23          |
| (1,3017) | 1:12:A:VAL:H     | 1:14:A:PRO:HD3   | 6        | 0.23          |
| (1,2999) | 1:140:A:LYS:H    | 1:141:A:TYR:HB2  | 4        | 0.23          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB2   | 13       | 0.23          |
| (1,2887) | 1:133:A:ARG:H    | 1:131:A:ILE:HG21 | 16       | 0.23          |
| (1,2868) | 1:12:A:VAL:H     | 1:10:A:LEU:HG    | 14       | 0.23          |
| (1,2842) | 1:140:A:LYS:H    | 1:139:A:GLU:HB2  | 14       | 0.23          |
| (1,2809) | 1:132:A:GLU:H    | 1:131:A:ILE:HG22 | 15       | 0.23          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG22  | 19       | 0.23          |
| (1,2725) | 1:38:A:THR:H     | 1:38:A:THR:HG23  | 20       | 0.23          |
| (1,2582) | 1:51:A:GLN:H     | 1:48:A:SER:HB2   | 10       | 0.23          |
| (1,2582) | 1:51:A:GLN:H     | 1:48:A:SER:HB2   | 19       | 0.23          |
| (1,2556) | 1:40:A:GLN:H     | 1:93:A:THR:HG23  | 15       | 0.23          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG2  | 12       | 0.23          |
| (1,2503) | 1:31:A:LYS:H     | 1:30:A:ILE:HG12  | 19       | 0.23          |
| (1,2412) | 1:102:A:LEU:H    | 1:118:A:THR:HG22 | 12       | 0.23          |
| (1,2387) | 1:29:A:LEU:HD13  | 1:92:A:VAL:HG11  | 15       | 0.23          |
| (1,2344) | 1:253:A:ILE:HA   | 1:255:A:GLU:HG2  | 13       | 0.23          |
| (1,2344) | 1:253:A:ILE:HA   | 1:254:A:GLU:HG3  | 20       | 0.23          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB2   | 9        | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 9        | 0.23          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 9        | 0.23          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 17       | 0.23          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3   | 17       | 0.23          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3   | 17       | 0.23          |
| (1,2169) | 1:56:A:ILE:HG22 | 1:58:A:VAL:HB    | 18       | 0.23          |
| (1,1455) | 1:51:A:GLN:HG2  | 1:51:A:GLN:H     | 9        | 0.23          |
| (1,1455) | 1:51:A:GLN:HG3  | 1:51:A:GLN:H     | 9        | 0.23          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG21  | 1        | 0.23          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG22  | 1        | 0.23          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG23  | 1        | 0.23          |
| (1,3192) | 1:13:A:ALA:H    | 1:12:A:VAL:HG23  | 20       | 0.22          |
| (1,3175) | 1:64:A:ALA:HB3  | 1:149:A:ARG:HD3  | 3        | 0.22          |
| (1,3174) | 1:70:A:ASN:HD21 | 1:126:A:LEU:HB3  | 19       | 0.22          |
| (1,3158) | 1:108:A:ASP:HB2 | 1:80:A:ILE:HD11  | 17       | 0.22          |
| (1,3135) | 1:83:A:ALA:H    | 1:82:A:PRO:HB3   | 16       | 0.22          |
| (1,3128) | 1:141:A:TYR:HD2 | 1:137:A:GLU:HG2  | 17       | 0.22          |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H     | 6        | 0.22          |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H     | 19       | 0.22          |
| (1,3065) | 1:92:A:VAL:HG13 | 1:93:A:THR:H     | 14       | 0.22          |
| (1,3065) | 1:92:A:VAL:HG12 | 1:93:A:THR:H     | 17       | 0.22          |
| (1,3008) | 1:148:A:GLN:H   | 1:151:A:ARG:HB2  | 10       | 0.22          |
| (1,2918) | 1:45:A:THR:H    | 1:158:A:LEU:HG   | 16       | 0.22          |
| (1,2918) | 1:45:A:THR:H    | 1:158:A:LEU:HG   | 17       | 0.22          |
| (1,2887) | 1:133:A:ARG:H   | 1:131:A:ILE:HG23 | 12       | 0.22          |
| (1,2604) | 1:43:A:ILE:H    | 1:43:A:ILE:HD13  | 7        | 0.22          |
| (1,2567) | 1:113:A:LYS:H   | 1:114:A:ALA:HB3  | 18       | 0.22          |
| (1,2567) | 1:113:A:LYS:H   | 1:114:A:ALA:HB2  | 19       | 0.22          |
| (1,2549) | 1:95:A:ASP:H    | 1:93:A:THR:HG21  | 9        | 0.22          |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG2  | 13       | 0.22          |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG21  | 1        | 0.22          |
| (1,2524) | 1:42:A:GLN:H    | 1:44:A:PHE:HD1   | 8        | 0.22          |
| (1,2516) | 1:96:A:ILE:H    | 1:39:A:LYS:HB2   | 4        | 0.22          |
| (1,2503) | 1:31:A:LYS:H    | 1:30:A:ILE:HG12  | 10       | 0.22          |
| (1,2502) | 1:31:A:LYS:H    | 1:30:A:ILE:HG12  | 10       | 0.22          |
| (1,2501) | 1:31:A:LYS:H    | 1:28:A:ALA:HB3   | 1        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2501) | 1:31:A:LYS:H     | 1:28:A:ALA:HB2   | 3        | 0.22          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD12 | 5        | 0.22          |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD11 | 20       | 0.22          |
| (1,2425) | 1:91:A:GLU:H     | 1:90:A:ILE:HG12  | 1        | 0.22          |
| (1,2407) | 1:102:A:LEU:H    | 1:101:A:ILE:HG22 | 7        | 0.22          |
| (1,2368) | 1:115:A:ASN:HA   | 1:75:A:PHE:HE2   | 4        | 0.22          |
| (1,2344) | 1:253:A:ILE:HA   | 1:255:A:GLU:HG2  | 12       | 0.22          |
| (1,2278) | 1:140:A:LYS:HB2  | 1:137:A:GLU:HG2  | 2        | 0.22          |
| (1,2182) | 1:54:A:VAL:HG23  | 1:77:A:LEU:HA    | 20       | 0.22          |
| (1,2169) | 1:56:A:ILE:HG23  | 1:58:A:VAL:HB    | 6        | 0.22          |
| (1,2169) | 1:56:A:ILE:HG21  | 1:58:A:VAL:HB    | 12       | 0.22          |
| (1,2144) | 1:27:A:THR:HG23  | 1:42:A:GLN:HE22  | 19       | 0.22          |
| (1,2109) | 1:66:A:THR:HG22  | 1:27:A:THR:H     | 1        | 0.22          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22  | 9        | 0.21          |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22  | 18       | 0.21          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB3   | 8        | 0.21          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB1   | 14       | 0.21          |
| (1,3137) | 1:158:A:LEU:HD22 | 1:21:A:THR:HA    | 10       | 0.21          |
| (1,3125) | 1:75:A:PHE:HD2   | 1:117:A:ILE:HG23 | 9        | 0.21          |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H     | 15       | 0.21          |
| (1,2967) | 1:99:A:ASN:H     | 1:36:A:ILE:HD11  | 9        | 0.21          |
| (1,2949) | 1:69:A:ASN:H     | 1:68:A:ASP:HB2   | 6        | 0.21          |
| (1,2936) | 1:65:A:MET:H     | 1:63:A:ARG:HA    | 11       | 0.21          |
| (1,2931) | 1:62:A:GLU:H     | 1:62:A:GLU:HG3   | 3        | 0.21          |
| (1,2931) | 1:62:A:GLU:H     | 1:26:A:MET:HG3   | 6        | 0.21          |
| (1,2918) | 1:45:A:THR:H     | 1:158:A:LEU:HG   | 9        | 0.21          |
| (1,2918) | 1:45:A:THR:H     | 1:158:A:LEU:HG   | 11       | 0.21          |
| (1,2918) | 1:45:A:THR:H     | 1:158:A:LEU:HG   | 20       | 0.21          |
| (1,2824) | 1:146:A:GLU:H    | 1:143:A:ALA:HA   | 16       | 0.21          |
| (1,2809) | 1:132:A:GLU:H    | 1:131:A:ILE:HG21 | 7        | 0.21          |
| (1,2800) | 1:34:A:SER:H     | 1:13:A:ALA:HB1   | 18       | 0.21          |
| (1,2716) | 1:19:A:LEU:H     | 1:28:A:ALA:HB2   | 1        | 0.21          |
| (1,2649) | 1:100:A:GLY:H    | 1:98:A:ALA:HB3   | 13       | 0.21          |
| (1,2649) | 1:100:A:GLY:H    | 1:98:A:ALA:HB2   | 19       | 0.21          |
| (1,2582) | 1:51:A:GLN:H     | 1:48:A:SER:HB2   | 2        | 0.21          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG2  | 3        | 0.21          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG2  | 11       | 0.21          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG2  | 19       | 0.21          |
| (1,2429) | 1:27:A:THR:H     | 1:26:A:MET:HE1   | 19       | 0.21          |
| (1,2420) | 1:119:A:ILE:H    | 1:101:A:ILE:HG21 | 4        | 0.21          |
| (1,2420) | 1:119:A:ILE:H    | 1:101:A:ILE:HG21 | 8        | 0.21          |
| (1,2391) | 1:15:A:LEU:HD21  | 1:14:A:PRO:HD2   | 18       | 0.21          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2374) | 1:14:A:PRO:HD2  | 1:15:A:LEU:HD21  | 18       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3  | 13       | 0.21          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3  | 13       | 0.21          |
| (1,2256) | 1:94:A:PHE:HE2  | 1:19:A:LEU:HB3   | 1        | 0.21          |
| (1,2010) | 1:9:A:LEU:HA    | 1:9:A:LEU:HD23   | 7        | 0.21          |
| (1,1455) | 1:51:A:GLN:HG2  | 1:51:A:GLN:H     | 14       | 0.21          |
| (1,1455) | 1:51:A:GLN:HG3  | 1:51:A:GLN:H     | 14       | 0.21          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG21  | 5        | 0.21          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG22  | 5        | 0.21          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG23  | 5        | 0.21          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG21  | 5        | 0.21          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG22  | 5        | 0.21          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG23  | 5        | 0.21          |
| (1,3157) | 1:24:A:GLY:H    | 1:152:A:VAL:HB   | 2        | 0.2           |
| (1,3156) | 1:70:A:ASN:H    | 1:15:A:LEU:HG    | 3        | 0.2           |
| (1,3155) | 1:14:A:PRO:HA   | 1:13:A:ALA:HB1   | 19       | 0.2           |
| (1,3149) | 1:13:A:ALA:HB2  | 1:14:A:PRO:HD2   | 17       | 0.2           |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H     | 9        | 0.2           |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H     | 14       | 0.2           |
| (1,2960) | 1:86:A:GLY:H    | 1:87:A:VAL:HG21  | 10       | 0.2           |
| (1,2947) | 1:69:A:ASN:H    | 1:69:A:ASN:HD22  | 2        | 0.2           |
| (1,2944) | 1:68:A:ASP:H    | 1:68:A:ASP:HB2   | 7        | 0.2           |
| (1,2824) | 1:146:A:GLU:H   | 1:143:A:ALA:HA   | 6        | 0.2           |
| (1,2716) | 1:19:A:LEU:H    | 1:28:A:ALA:HB1   | 10       | 0.2           |
| (1,2539) | 1:32:A:ARG:H    | 1:31:A:LYS:HB3   | 19       | 0.2           |
| (1,2447) | 1:97:A:ASP:H    | 1:101:A:ILE:HD11 | 3        | 0.2           |
| (1,2430) | 1:27:A:THR:H    | 1:29:A:LEU:HD11  | 14       | 0.2           |
| (1,2427) | 1:91:A:GLU:H    | 1:90:A:ILE:HD13  | 6        | 0.2           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2425) | 1:91:A:GLU:H    | 1:90:A:ILE:HG12  | 10       | 0.2           |
| (1,2425) | 1:91:A:GLU:H    | 1:90:A:ILE:HG12  | 13       | 0.2           |
| (1,2425) | 1:91:A:GLU:H    | 1:106:A:ALA:HB3  | 16       | 0.2           |
| (1,2412) | 1:102:A:LEU:H   | 1:118:A:THR:HG22 | 2        | 0.2           |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 15       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3  | 15       | 0.2           |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3  | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 9        | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 15       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 15       | 0.2           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 17       | 0.2           |
| (1,2247) | 1:10:A:LEU:HD13  | 1:10:A:LEU:HA   | 17       | 0.2           |
| (1,2175) | 1:26:A:MET:HE3   | 1:16:A:SER:HA   | 2        | 0.2           |
| (1,2020) | 1:72:A:LEU:HA    | 1:72:A:LEU:HD12 | 10       | 0.2           |
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB2 | 6        | 0.2           |
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB3 | 6        | 0.2           |
| (1,504)  | 1:39:A:LYS:HB2   | 1:39:A:LYS:HE2  | 7        | 0.2           |
| (1,504)  | 1:39:A:LYS:HB2   | 1:39:A:LYS:HE3  | 7        | 0.2           |
| (1,504)  | 1:39:A:LYS:HB3   | 1:39:A:LYS:HE2  | 7        | 0.2           |
| (1,504)  | 1:39:A:LYS:HB3   | 1:39:A:LYS:HE3  | 7        | 0.2           |
| (1,141)  | 1:103:A:ASN:HD21 | 1:119:A:ILE:HA  | 19       | 0.2           |
| (1,141)  | 1:103:A:ASN:HD22 | 1:119:A:ILE:HA  | 19       | 0.2           |
| (1,3192) | 1:13:A:ALA:H     | 1:12:A:VAL:HG22 | 4        | 0.19          |
| (1,3177) | 1:26:A:MET:HE2   | 1:29:A:LEU:H    | 4        | 0.19          |
| (1,3157) | 1:24:A:GLY:H     | 1:159:A:GLU:HG3 | 5        | 0.19          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB2  | 1        | 0.19          |
| (1,3135) | 1:83:A:ALA:H     | 1:82:A:PRO:HB2  | 6        | 0.19          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H    | 1        | 0.19          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H    | 4        | 0.19          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H    | 13       | 0.19          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H    | 14       | 0.19          |
| (1,3065) | 1:92:A:VAL:HG11  | 1:93:A:THR:H    | 3        | 0.19          |
| (1,3011) | 1:157:A:ALA:H    | 1:158:A:LEU:HG  | 15       | 0.19          |
| (1,2999) | 1:140:A:LYS:H    | 1:141:A:TYR:HB2 | 1        | 0.19          |
| (1,2946) | 1:68:A:ASP:H     | 1:69:A:ASN:HA   | 1        | 0.19          |
| (1,2946) | 1:68:A:ASP:H     | 1:69:A:ASN:HA   | 19       | 0.19          |
| (1,2917) | 1:43:A:ILE:H     | 1:44:A:PHE:HD2  | 1        | 0.19          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2916) | 1:96:A:ILE:H    | 1:39:A:LYS:HG3   | 2        | 0.19          |
| (1,2913) | 1:38:A:THR:H    | 1:37:A:PRO:HG3   | 14       | 0.19          |
| (1,2904) | 1:18:A:GLY:H    | 1:19:A:LEU:HD22  | 4        | 0.19          |
| (1,2790) | 1:15:A:LEU:H    | 1:14:A:PRO:HG2   | 15       | 0.19          |
| (1,2688) | 1:45:A:THR:H    | 1:45:A:THR:HG23  | 9        | 0.19          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB1   | 15       | 0.19          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB2   | 20       | 0.19          |
| (1,2582) | 1:51:A:GLN:H    | 1:48:A:SER:HB2   | 1        | 0.19          |
| (1,2567) | 1:113:A:LYS:H   | 1:111:A:THR:HG23 | 5        | 0.19          |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG3  | 15       | 0.19          |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG2  | 18       | 0.19          |
| (1,2503) | 1:31:A:LYS:H    | 1:30:A:ILE:HG12  | 12       | 0.19          |
| (1,2502) | 1:31:A:LYS:H    | 1:30:A:ILE:HG12  | 12       | 0.19          |
| (1,2429) | 1:27:A:THR:H    | 1:25:A:VAL:HB    | 1        | 0.19          |
| (1,2420) | 1:119:A:ILE:H   | 1:101:A:ILE:HG21 | 3        | 0.19          |
| (1,2412) | 1:102:A:LEU:H   | 1:118:A:THR:HG21 | 3        | 0.19          |
| (1,2412) | 1:102:A:LEU:H   | 1:118:A:THR:HG22 | 7        | 0.19          |
| (1,2278) | 1:140:A:LYS:HB3 | 1:137:A:GLU:HG2  | 14       | 0.19          |
| (1,2188) | 1:80:A:ILE:HG22 | 1:53:A:GLY:HA2   | 14       | 0.19          |
| (1,2169) | 1:56:A:ILE:HG23 | 1:58:A:VAL:HB    | 8        | 0.19          |
| (1,2144) | 1:27:A:THR:HG22 | 1:42:A:GLN:HE22  | 5        | 0.19          |
| (1,2109) | 1:66:A:THR:HG22 | 1:27:A:THR:H     | 6        | 0.19          |
| (1,1491) | 1:17:A:LEU:HD11 | 1:18:A:GLY:H     | 18       | 0.19          |
| (1,1491) | 1:17:A:LEU:HD12 | 1:18:A:GLY:H     | 18       | 0.19          |
| (1,1491) | 1:17:A:LEU:HD13 | 1:18:A:GLY:H     | 18       | 0.19          |
| (1,1491) | 1:17:A:LEU:HD21 | 1:18:A:GLY:H     | 18       | 0.19          |
| (1,1491) | 1:17:A:LEU:HD22 | 1:18:A:GLY:H     | 18       | 0.19          |
| (1,1491) | 1:17:A:LEU:HD23 | 1:18:A:GLY:H     | 18       | 0.19          |
| (1,1455) | 1:51:A:GLN:HG2  | 1:51:A:GLN:H     | 5        | 0.19          |
| (1,1455) | 1:51:A:GLN:HG3  | 1:51:A:GLN:H     | 5        | 0.19          |
| (1,1455) | 1:51:A:GLN:HG2  | 1:51:A:GLN:H     | 15       | 0.19          |
| (1,1455) | 1:51:A:GLN:HG3  | 1:51:A:GLN:H     | 15       | 0.19          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG21  | 6        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG22  | 6        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG23  | 6        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG21  | 6        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG22  | 6        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG23  | 6        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG21  | 7        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG22  | 7        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG23  | 7        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG21  | 7        | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,942)  | 1:37:A:PRO:HB3   | 1:38:A:THR:HG22  | 7        | 0.19          |
| (1,942)  | 1:37:A:PRO:HB3   | 1:38:A:THR:HG23  | 7        | 0.19          |
| (1,520)  | 1:120:A:THR:HA   | 1:99:A:ASN:HB2   | 19       | 0.19          |
| (1,520)  | 1:120:A:THR:HA   | 1:99:A:ASN:HB3   | 19       | 0.19          |
| (1,272)  | 1:129:A:GLU:H    | 1:127:A:SER:HA   | 11       | 0.19          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 12       | 0.18          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB3   | 7        | 0.18          |
| (1,3149) | 1:13:A:ALA:HB3   | 1:14:A:PRO:HD2   | 8        | 0.18          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB3   | 4        | 0.18          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 20       | 0.18          |
| (1,3065) | 1:92:A:VAL:HG13  | 1:93:A:THR:H     | 5        | 0.18          |
| (1,3065) | 1:92:A:VAL:HG13  | 1:93:A:THR:H     | 7        | 0.18          |
| (1,3026) | 1:141:A:TYR:H    | 1:138:A:ALA:HB3  | 14       | 0.18          |
| (1,2950) | 1:69:A:ASN:H     | 1:67:A:LYS:HG3   | 16       | 0.18          |
| (1,2931) | 1:62:A:GLU:H     | 1:62:A:GLU:HG2   | 4        | 0.18          |
| (1,2918) | 1:45:A:THR:H     | 1:158:A:LEU:HG   | 14       | 0.18          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG3   | 9        | 0.18          |
| (1,2842) | 1:140:A:LYS:H    | 1:139:A:GLU:HB2  | 11       | 0.18          |
| (1,2809) | 1:132:A:GLU:H    | 1:131:A:ILE:HG22 | 1        | 0.18          |
| (1,2809) | 1:132:A:GLU:H    | 1:131:A:ILE:HG22 | 2        | 0.18          |
| (1,2749) | 1:11:A:ASP:H     | 1:10:A:LEU:HD13  | 14       | 0.18          |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG21  | 13       | 0.18          |
| (1,2535) | 1:90:A:ILE:H     | 1:89:A:GLN:HG3   | 2        | 0.18          |
| (1,2527) | 1:104:A:VAL:H    | 1:75:A:PHE:HE1   | 8        | 0.18          |
| (1,2517) | 1:42:A:GLN:H     | 1:92:A:VAL:HG22  | 7        | 0.18          |
| (1,2425) | 1:91:A:GLU:H     | 1:106:A:ALA:HB2  | 9        | 0.18          |
| (1,2420) | 1:119:A:ILE:H    | 1:101:A:ILE:HG22 | 9        | 0.18          |
| (1,2392) | 1:36:A:ILE:HD13  | 1:14:A:PRO:HD3   | 16       | 0.18          |
| (1,2381) | 1:104:A:VAL:HG13 | 1:19:A:LEU:HG    | 11       | 0.18          |
| (1,2301) | 1:85:A:ARG:HD2   | 1:85:A:ARG:HB2   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD2   | 1:85:A:ARG:HB2   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD2   | 1:85:A:ARG:HB3   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD2   | 1:85:A:ARG:HB3   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD2   | 1:85:A:ARG:HB2   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD2   | 1:85:A:ARG:HB2   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD2   | 1:85:A:ARG:HB3   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD2   | 1:85:A:ARG:HB3   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB2   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB2   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB3   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB3   | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB2   | 7        | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2 | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3 | 7        | 0.18          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3 | 7        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 1        | 0.18          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2 | 1        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD2   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD2   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD2   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG22  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD2   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2250) | 1:87:A:VAL:HG23  | 1:84:A:PRO:HD3   | 1        | 0.18          |
| (1,2154) | 1:104:A:VAL:HG12 | 1:75:A:PHE:HE2   | 12       | 0.18          |
| (1,1971) | 1:43:A:ILE:HD12  | 1:92:A:VAL:H     | 18       | 0.18          |
| (1,1967) | 1:80:A:ILE:HD13  | 1:54:A:VAL:HA    | 2        | 0.18          |
| (1,1963) | 1:80:A:ILE:HD12  | 1:52:A:PRO:HA    | 16       | 0.18          |
| (1,1785) | 1:67:A:LYS:HA    | 1:69:A:ASN:H     | 17       | 0.18          |
| (1,1455) | 1:51:A:GLN:HG2   | 1:51:A:GLN:H     | 8        | 0.18          |
| (1,1455) | 1:51:A:GLN:HG3   | 1:51:A:GLN:H     | 8        | 0.18          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB3   | 18       | 0.17          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB1   | 6        | 0.17          |
| (1,3145) | 1:87:A:VAL:HA    | 1:83:A:ALA:HB3   | 20       | 0.17          |
| (1,3125) | 1:75:A:PHE:HD1   | 1:117:A:ILE:HG23 | 10       | 0.17          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 2        | 0.17          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 5        | 0.17          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 12       | 0.17          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 16       | 0.17          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 17       | 0.17          |
| (1,3089) | 1:35:A:THR:HB    | 1:36:A:ILE:H     | 19       | 0.17          |
| (1,2996) | 1:146:A:GLU:H    | 1:142:A:LYS:HG2  | 7        | 0.17          |
| (1,2972) | 1:104:A:VAL:H    | 1:117:A:ILE:HG12 | 3        | 0.17          |
| (1,2969) | 1:100:A:GLY:H    | 1:101:A:ILE:HD11 | 18       | 0.17          |
| (1,2967) | 1:99:A:ASN:H     | 1:36:A:ILE:HD11  | 3        | 0.17          |
| (1,2944) | 1:68:A:ASP:H     | 1:68:A:ASP:HB2   | 8        | 0.17          |
| (1,2931) | 1:62:A:GLU:H     | 1:62:A:GLU:HG3   | 12       | 0.17          |
| (1,2921) | 1:48:A:SER:H     | 1:85:A:ARG:HG2   | 12       | 0.17          |
| (1,2851) | 1:126:A:LEU:H    | 1:131:A:ILE:HD12 | 15       | 0.17          |
| (1,2844) | 1:118:A:THR:H    | 1:116:A:LYS:HD2  | 8        | 0.17          |
| (1,2824) | 1:146:A:GLU:H    | 1:143:A:ALA:HA   | 11       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2824) | 1:146:A:GLU:H    | 1:143:A:ALA:HA   | 12       | 0.17          |
| (1,2824) | 1:146:A:GLU:H    | 1:142:A:LYS:HA   | 20       | 0.17          |
| (1,2805) | 1:132:A:GLU:H    | 1:129:A:GLU:HA   | 17       | 0.17          |
| (1,2748) | 1:11:A:ASP:H     | 1:36:A:ILE:HG12  | 4        | 0.17          |
| (1,2743) | 1:135:A:VAL:H    | 1:134:A:MET:HG2  | 1        | 0.17          |
| (1,2712) | 1:137:A:GLU:H    | 1:138:A:ALA:HB3  | 11       | 0.17          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG21  | 17       | 0.17          |
| (1,2582) | 1:51:A:GLN:H     | 1:48:A:SER:HB2   | 12       | 0.17          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG3  | 17       | 0.17          |
| (1,2526) | 1:42:A:GLN:H     | 1:94:A:PHE:H     | 7        | 0.17          |
| (1,2425) | 1:91:A:GLU:H     | 1:90:A:ILE:HG12  | 7        | 0.17          |
| (1,2425) | 1:91:A:GLU:H     | 1:90:A:ILE:HG12  | 18       | 0.17          |
| (1,2412) | 1:102:A:LEU:H    | 1:118:A:THR:HG21 | 20       | 0.17          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG23  | 4        | 0.17          |
| (1,2404) | 1:92:A:VAL:H     | 1:41:A:THR:HG23  | 15       | 0.17          |
| (1,2392) | 1:36:A:ILE:HD13  | 1:14:A:PRO:HD3   | 20       | 0.17          |
| (1,2388) | 1:19:A:LEU:HD23  | 1:57:A:GLN:H     | 18       | 0.17          |
| (1,2381) | 1:104:A:VAL:HG11 | 1:19:A:LEU:HG    | 19       | 0.17          |
| (1,2368) | 1:115:A:ASN:HA   | 1:75:A:PHE:HE1   | 7        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD11  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD12  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD12  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD12  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD12  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD12  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD12  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD12  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD12  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD13  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD13  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD13  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD13  | 1:74:A:ARG:HB3   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD13  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD13  | 1:74:A:ARG:HB2   | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD13  | 1:74:A:ARG:HB3   | 1        | 0.17          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3 | 1        | 0.17          |
| (1,2256) | 1:44:A:PHE:HD1  | 1:19:A:LEU:HB2 | 9        | 0.17          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 15       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 15       | 0.17          |
| (1,2224) | 1:44:A:PHE:H    | 1:43:A:ILE:HD12 | 18       | 0.17          |
| (1,2175) | 1:26:A:MET:HE3  | 1:16:A:SER:HA   | 5        | 0.17          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 3        | 0.17          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 3        | 0.17          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 3        | 0.17          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 9        | 0.17          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 9        | 0.17          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 9        | 0.17          |
| (1,1752) | 1:22:A:ALA:HB1  | 1:47:A:TYR:H    | 8        | 0.17          |
| (1,1752) | 1:22:A:ALA:HB2  | 1:47:A:TYR:H    | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1752) | 1:22:A:ALA:HB3  | 1:47:A:TYR:H     | 8        | 0.17          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG21  | 13       | 0.17          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG22  | 13       | 0.17          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG23  | 13       | 0.17          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG21  | 15       | 0.17          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG22  | 15       | 0.17          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG23  | 15       | 0.17          |
| (1,94)   | 1:253:A:ILE:HB  | 1:253:A:ILE:HA   | 20       | 0.17          |
| (1,3177) | 1:26:A:MET:HE3  | 1:29:A:LEU:H     | 14       | 0.16          |
| (1,3172) | 1:56:A:ILE:HD11 | 1:77:A:LEU:HA    | 19       | 0.16          |
| (1,3165) | 1:96:A:ILE:HG22 | 1:38:A:THR:H     | 19       | 0.16          |
| (1,3156) | 1:70:A:ASN:H    | 1:126:A:LEU:HD12 | 18       | 0.16          |
| (1,3128) | 1:141:A:TYR:HD2 | 1:144:A:GLU:HG3  | 1        | 0.16          |
| (1,3128) | 1:141:A:TYR:HD2 | 1:144:A:GLU:HG3  | 11       | 0.16          |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H     | 3        | 0.16          |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H     | 10       | 0.16          |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H     | 15       | 0.16          |
| (1,3045) | 1:33:A:ASN:HA   | 1:13:A:ALA:H     | 10       | 0.16          |
| (1,3036) | 1:114:A:ALA:H   | 1:108:A:ASP:H    | 10       | 0.16          |
| (1,3011) | 1:157:A:ALA:H   | 1:158:A:LEU:HG   | 1        | 0.16          |
| (1,3008) | 1:148:A:GLN:H   | 1:151:A:ARG:HB2  | 9        | 0.16          |
| (1,2972) | 1:104:A:VAL:H   | 1:117:A:ILE:HG12 | 1        | 0.16          |
| (1,2940) | 1:67:A:LYS:H    | 1:68:A:ASP:HB2   | 11       | 0.16          |
| (1,2833) | 1:116:A:LYS:H   | 1:75:A:PHE:HE1   | 15       | 0.16          |
| (1,2776) | 1:20:A:GLU:H    | 1:56:A:ILE:HG21  | 4        | 0.16          |
| (1,2765) | 1:139:A:GLU:H   | 1:139:A:GLU:HB3  | 4        | 0.16          |
| (1,2725) | 1:38:A:THR:H    | 1:38:A:THR:HG23  | 16       | 0.16          |
| (1,2684) | 1:158:A:LEU:H   | 1:90:A:ILE:HG13  | 3        | 0.16          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB1   | 9        | 0.16          |
| (1,2642) | 1:46:A:THR:H    | 1:45:A:THR:HG22  | 3        | 0.16          |
| (1,2604) | 1:43:A:ILE:H    | 1:43:A:ILE:HD11  | 20       | 0.16          |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG2  | 9        | 0.16          |
| (1,2543) | 1:114:A:ALA:H   | 1:113:A:LYS:HG3  | 20       | 0.16          |
| (1,2539) | 1:32:A:ARG:H    | 1:31:A:LYS:HB3   | 15       | 0.16          |
| (1,2495) | 1:57:A:GLN:H    | 1:55:A:LEU:HB3   | 3        | 0.16          |
| (1,2463) | 1:108:A:ASP:H   | 1:77:A:LEU:HG    | 19       | 0.16          |
| (1,2425) | 1:91:A:GLU:H    | 1:90:A:ILE:HG12  | 12       | 0.16          |
| (1,2412) | 1:102:A:LEU:H   | 1:118:A:THR:HG22 | 8        | 0.16          |
| (1,2344) | 1:253:A:ILE:HA  | 1:254:A:GLU:HG2  | 17       | 0.16          |
| (1,2256) | 1:94:A:PHE:HE1  | 1:19:A:LEU:HB2   | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2   | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2   | 6        | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 6        | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 6        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 9        | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 9        | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 11       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 11       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 12       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 12       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 13       | 0.16          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 13       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 14       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3  | 14       | 0.16          |
| (1,1967) | 1:80:A:ILE:HD12 | 1:54:A:VAL:HA   | 13       | 0.16          |
| (1,1967) | 1:80:A:ILE:HD13 | 1:54:A:VAL:HA   | 19       | 0.16          |
| (1,1963) | 1:80:A:ILE:HD12 | 1:77:A:LEU:HA   | 4        | 0.16          |
| (1,1954) | 1:96:A:ILE:HD13 | 1:100:A:GLY:HA2 | 5        | 0.16          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 5        | 0.16          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 5        | 0.16          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 5        | 0.16          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2 | 3        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB3  | 3        | 0.16          |
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB2  | 5        | 0.16          |
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB3  | 5        | 0.16          |
| (1,1908) | 1:21:A:THR:H     | 1:19:A:LEU:HD11  | 2        | 0.16          |
| (1,1908) | 1:21:A:THR:H     | 1:19:A:LEU:HD12  | 2        | 0.16          |
| (1,1908) | 1:21:A:THR:H     | 1:19:A:LEU:HD13  | 2        | 0.16          |
| (1,1908) | 1:21:A:THR:H     | 1:19:A:LEU:HD21  | 2        | 0.16          |
| (1,1908) | 1:21:A:THR:H     | 1:19:A:LEU:HD22  | 2        | 0.16          |
| (1,1908) | 1:21:A:THR:H     | 1:19:A:LEU:HD23  | 2        | 0.16          |
| (1,1673) | 1:116:A:LYS:HB2  | 1:116:A:LYS:H    | 12       | 0.16          |
| (1,1673) | 1:116:A:LYS:HB3  | 1:116:A:LYS:H    | 12       | 0.16          |
| (1,1673) | 1:116:A:LYS:HB2  | 1:116:A:LYS:H    | 13       | 0.16          |
| (1,1673) | 1:116:A:LYS:HB3  | 1:116:A:LYS:H    | 13       | 0.16          |
| (1,1106) | 1:35:A:THR:HG21  | 1:34:A:SER:HA    | 4        | 0.16          |
| (1,1106) | 1:35:A:THR:HG22  | 1:34:A:SER:HA    | 4        | 0.16          |
| (1,1106) | 1:35:A:THR:HG23  | 1:34:A:SER:HA    | 4        | 0.16          |
| (1,520)  | 1:120:A:THR:HA   | 1:99:A:ASN:HB2   | 11       | 0.16          |
| (1,520)  | 1:120:A:THR:HA   | 1:99:A:ASN:HB3   | 11       | 0.16          |
| (1,94)   | 1:253:A:ILE:HB   | 1:253:A:ILE:HA   | 16       | 0.16          |
| (1,3157) | 1:24:A:GLY:H     | 1:159:A:GLU:HG2  | 18       | 0.15          |
| (1,3130) | 1:141:A:TYR:HE2  | 1:144:A:GLU:HB2  | 3        | 0.15          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 11       | 0.15          |
| (1,3086) | 1:26:A:MET:HE2   | 1:19:A:LEU:H     | 20       | 0.15          |
| (1,3065) | 1:92:A:VAL:HG13  | 1:93:A:THR:H     | 19       | 0.15          |
| (1,3052) | 1:29:A:LEU:HD21  | 1:42:A:GLN:H     | 12       | 0.15          |
| (1,3026) | 1:141:A:TYR:H    | 1:140:A:LYS:HD2  | 6        | 0.15          |
| (1,3017) | 1:12:A:VAL:H     | 1:14:A:PRO:HD3   | 11       | 0.15          |
| (1,2904) | 1:18:A:GLY:H     | 1:29:A:LEU:HD13  | 14       | 0.15          |
| (1,2790) | 1:15:A:LEU:H     | 1:14:A:PRO:HG2   | 16       | 0.15          |
| (1,2717) | 1:19:A:LEU:H     | 1:29:A:LEU:HD11  | 5        | 0.15          |
| (1,2642) | 1:46:A:THR:H     | 1:45:A:THR:HG23  | 5        | 0.15          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG3  | 5        | 0.15          |
| (1,2543) | 1:114:A:ALA:H    | 1:113:A:LYS:HG3  | 7        | 0.15          |
| (1,2425) | 1:91:A:GLU:H     | 1:90:A:ILE:HG12  | 20       | 0.15          |
| (1,2387) | 1:29:A:LEU:HD22  | 1:92:A:VAL:HG12  | 17       | 0.15          |
| (1,2379) | 1:158:A:LEU:HD11 | 1:44:A:PHE:H     | 16       | 0.15          |
| (1,2365) | 1:70:A:ASN:HA    | 1:126:A:LEU:HD11 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA    | 1:126:A:LEU:HD11 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA    | 1:126:A:LEU:HD12 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA    | 1:126:A:LEU:HD12 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA    | 1:126:A:LEU:HD13 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA    | 1:126:A:LEU:HD13 | 8        | 0.15          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2365) | 1:70:A:ASN:HA   | 1:126:A:LEU:HD21 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA   | 1:126:A:LEU:HD21 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA   | 1:126:A:LEU:HD22 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA   | 1:126:A:LEU:HD22 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA   | 1:126:A:LEU:HD23 | 8        | 0.15          |
| (1,2365) | 1:70:A:ASN:HA   | 1:126:A:LEU:HD23 | 8        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 5        | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 15       | 0.15          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 15       | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2  | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2  | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3  | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3  | 1        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 1        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 4        | 0.15          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 4        | 0.15          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB2  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD11 | 1:55:A:LEU:HB3  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2  | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB2  | 19       | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD12 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD13 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD21 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD22 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB2 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2266) | 1:55:A:LEU:HD23 | 1:55:A:LEU:HB3 | 19       | 0.15          |
| (1,2256) | 1:94:A:PHE:HE2  | 1:19:A:LEU:HB2 | 3        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 4        | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 4        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 7        | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD11 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD12 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD13 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD21 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD22 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 7        | 0.15          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB2 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2254) | 1:17:A:LEU:HD23 | 1:17:A:LEU:HB3 | 7        | 0.15          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3 | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2 | 14       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 14       | 0.15          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 14       | 0.15          |
| (1,2182) | 1:54:A:VAL:HG23 | 1:76:A:GLU:HA   | 6        | 0.15          |
| (1,2175) | 1:26:A:MET:HE3  | 1:16:A:SER:HA   | 15       | 0.15          |
| (1,2169) | 1:56:A:ILE:HG21 | 1:58:A:VAL:HB   | 17       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD11 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD11 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD12 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD12 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD13 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD13 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD21 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD21 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD22 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD22 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD23 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD23 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD21 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD21 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD22 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD22 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD23 | 18       | 0.15          |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD23 | 18       | 0.15          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2 | 1        | 0.15          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB3 | 1        | 0.15          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2 | 2        | 0.15          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB3 | 2        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2 | 8        | 0.15          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB3 | 8        | 0.15          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2 | 15       | 0.15          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB3 | 15       | 0.15          |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 11       | 0.15          |
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 11       | 0.15          |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 17       | 0.15          |
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 17       | 0.15          |
| (1,1621) | 1:67:A:LYS:HG2  | 1:68:A:ASP:H    | 6        | 0.15          |
| (1,1621) | 1:67:A:LYS:HG3  | 1:68:A:ASP:H    | 6        | 0.15          |
| (1,1612) | 1:38:A:THR:HB   | 1:39:A:LYS:H    | 18       | 0.15          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG21 | 20       | 0.15          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG22 | 20       | 0.15          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG23 | 20       | 0.15          |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB2  | 3        | 0.15          |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB3  | 3        | 0.15          |
| (1,405)  | 1:39:A:LYS:HD2  | 1:95:A:ASP:HA   | 1        | 0.15          |
| (1,405)  | 1:39:A:LYS:HD3  | 1:95:A:ASP:HA   | 1        | 0.15          |
| (1,94)   | 1:253:A:ILE:HB  | 1:253:A:ILE:HA  | 1        | 0.15          |
| (1,3180) | 1:35:A:THR:HA   | 1:36:A:ILE:HG12 | 10       | 0.14          |
| (1,3177) | 1:26:A:MET:HE2  | 1:29:A:LEU:H    | 12       | 0.14          |
| (1,3157) | 1:24:A:GLY:H    | 1:152:A:VAL:HB  | 20       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 15       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 15       | 0.14          |
| (1,3090) | 1:36:A:ILE:HB   | 1:36:A:ILE:H    | 18       | 0.14          |
| (1,3042) | 1:19:A:LEU:HD13 | 1:59:A:TYR:H    | 15       | 0.14          |
| (1,3017) | 1:12:A:VAL:H    | 1:14:A:PRO:HD3  | 15       | 0.14          |
| (1,2980) | 1:111:A:THR:H   | 1:81:A:PRO:HG3  | 19       | 0.14          |
| (1,2979) | 1:110:A:SER:H   | 1:80:A:ILE:HG13 | 4        | 0.14          |
| (1,2950) | 1:69:A:ASN:H    | 1:67:A:LYS:HG3  | 12       | 0.14          |
| (1,2924) | 1:54:A:VAL:H    | 1:77:A:LEU:HD22 | 2        | 0.14          |
| (1,2913) | 1:38:A:THR:H    | 1:37:A:PRO:HG3  | 3        | 0.14          |
| (1,2904) | 1:18:A:GLY:H    | 1:19:A:LEU:HD21 | 2        | 0.14          |
| (1,2761) | 1:30:A:ILE:H    | 1:30:A:ILE:HD12 | 12       | 0.14          |
| (1,2727) | 1:38:A:THR:H    | 1:36:A:ILE:HG23 | 19       | 0.14          |
| (1,2696) | 1:127:A:SER:H   | 1:127:A:SER:HA  | 18       | 0.14          |
| (1,2675) | 1:76:A:GLU:H    | 1:55:A:LEU:HD12 | 2        | 0.14          |
| (1,2613) | 1:9:A:LEU:HA    | 1:9:A:LEU:H     | 15       | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2613) | 1:9:A:LEU:HA    | 1:9:A:LEU:H      | 19       | 0.14          |
| (1,2613) | 1:9:A:LEU:HA    | 1:9:A:LEU:H      | 20       | 0.14          |
| (1,2567) | 1:113:A:LYS:H   | 1:111:A:THR:HG21 | 3        | 0.14          |
| (1,2567) | 1:113:A:LYS:H   | 1:114:A:ALA:HB3  | 12       | 0.14          |
| (1,2561) | 1:101:A:ILE:H   | 1:101:A:ILE:HD11 | 12       | 0.14          |
| (1,2549) | 1:95:A:ASP:H    | 1:93:A:THR:HG22  | 3        | 0.14          |
| (1,2463) | 1:108:A:ASP:H   | 1:77:A:LEU:HG    | 16       | 0.14          |
| (1,2447) | 1:97:A:ASP:H    | 1:101:A:ILE:HD13 | 10       | 0.14          |
| (1,2344) | 1:253:A:ILE:HA  | 1:254:A:GLU:HG2  | 15       | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 4        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB2   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD2  | 1:85:A:ARG:HB3   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB2   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 9        | 0.14          |
| (1,2301) | 1:85:A:ARG:HD3  | 1:85:A:ARG:HB3   | 9        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2  | 3        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 3        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 5        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 6        | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 6        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 7        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 8        | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 10       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 10       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 11       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 12       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 12       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 14       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 16       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 19       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 19       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE2 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD2 | 1:116:A:LYS:HE3 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE2 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 20       | 0.14          |
| (1,2270) | 1:116:A:LYS:HD3 | 1:116:A:LYS:HE3 | 20       | 0.14          |
| (1,2256) | 1:94:A:PHE:HE1  | 1:19:A:LEU:HB2  | 4        | 0.14          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 20       | 0.14          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3   | 20       | 0.14          |
| (1,2219) | 1:204:A:GLU:HA  | 1:203:A:ALA:H    | 19       | 0.14          |
| (1,2041) | 1:94:A:PHE:HA   | 1:92:A:VAL:HG11  | 16       | 0.14          |
| (1,2009) | 1:9:A:LEU:HA    | 1:9:A:LEU:H      | 15       | 0.14          |
| (1,2009) | 1:9:A:LEU:HA    | 1:9:A:LEU:H      | 19       | 0.14          |
| (1,2009) | 1:9:A:LEU:HA    | 1:9:A:LEU:H      | 20       | 0.14          |
| (1,1982) | 1:252:A:THR:HA  | 1:253:A:ILE:HG12 | 10       | 0.14          |
| (1,1963) | 1:80:A:ILE:HD13 | 1:77:A:LEU:HA    | 19       | 0.14          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2  | 14       | 0.14          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2  | 14       | 0.14          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2  | 14       | 0.14          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2  | 13       | 0.14          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB3  | 13       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB2  | 18       | 0.14          |
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB3  | 18       | 0.14          |
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB2  | 19       | 0.14          |
| (1,1920) | 1:21:A:THR:H     | 1:158:A:LEU:HB3  | 19       | 0.14          |
| (1,1744) | 1:39:A:LYS:HD2   | 1:39:A:LYS:H     | 18       | 0.14          |
| (1,1744) | 1:39:A:LYS:HD3   | 1:39:A:LYS:H     | 18       | 0.14          |
| (1,520)  | 1:120:A:THR:HA   | 1:99:A:ASN:HB2   | 12       | 0.14          |
| (1,520)  | 1:120:A:THR:HA   | 1:99:A:ASN:HB3   | 12       | 0.14          |
| (1,405)  | 1:39:A:LYS:HD2   | 1:95:A:ASP:HA    | 2        | 0.14          |
| (1,405)  | 1:39:A:LYS:HD3   | 1:95:A:ASP:HA    | 2        | 0.14          |
| (1,3161) | 1:36:A:ILE:HD13  | 1:13:A:ALA:H     | 1        | 0.13          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB1   | 4        | 0.13          |
| (1,3155) | 1:14:A:PRO:HA    | 1:13:A:ALA:HB2   | 6        | 0.13          |
| (1,3151) | 1:38:A:THR:HB    | 1:96:A:ILE:HG22  | 18       | 0.13          |
| (1,3135) | 1:83:A:ALA:H     | 1:82:A:PRO:HB3   | 5        | 0.13          |
| (1,3128) | 1:141:A:TYR:HD2  | 1:144:A:GLU:HG2  | 19       | 0.13          |
| (1,3118) | 1:131:A:ILE:HD12 | 1:70:A:ASN:HD21  | 1        | 0.13          |
| (1,3090) | 1:36:A:ILE:HB    | 1:36:A:ILE:H     | 8        | 0.13          |
| (1,3017) | 1:12:A:VAL:H     | 1:14:A:PRO:HD3   | 18       | 0.13          |
| (1,3011) | 1:157:A:ALA:H    | 1:158:A:LEU:HG   | 19       | 0.13          |
| (1,3008) | 1:148:A:GLN:H    | 1:149:A:ARG:HB3  | 8        | 0.13          |
| (1,2972) | 1:104:A:VAL:H    | 1:118:A:THR:HG21 | 7        | 0.13          |
| (1,2967) | 1:99:A:ASN:H     | 1:36:A:ILE:HD13  | 14       | 0.13          |
| (1,2946) | 1:68:A:ASP:H     | 1:69:A:ASN:HA    | 6        | 0.13          |
| (1,2944) | 1:68:A:ASP:H     | 1:68:A:ASP:HB2   | 1        | 0.13          |
| (1,2921) | 1:48:A:SER:H     | 1:85:A:ARG:HG3   | 8        | 0.13          |
| (1,2916) | 1:96:A:ILE:H     | 1:39:A:LYS:HG3   | 13       | 0.13          |
| (1,2868) | 1:12:A:VAL:H     | 1:10:A:LEU:HB3   | 13       | 0.13          |
| (1,2833) | 1:116:A:LYS:H    | 1:75:A:PHE:HE2   | 14       | 0.13          |
| (1,2820) | 1:136:A:GLN:H    | 1:135:A:VAL:HG13 | 1        | 0.13          |
| (1,2820) | 1:136:A:GLN:H    | 1:135:A:VAL:HG13 | 13       | 0.13          |
| (1,2817) | 1:134:A:MET:H    | 1:131:A:ILE:HG22 | 1        | 0.13          |
| (1,2649) | 1:100:A:GLY:H    | 1:98:A:ALA:HB2   | 1        | 0.13          |
| (1,2648) | 1:53:A:GLY:H     | 1:54:A:VAL:HG12  | 2        | 0.13          |
| (1,2582) | 1:51:A:GLN:H     | 1:48:A:SER:HB2   | 17       | 0.13          |
| (1,2524) | 1:42:A:GLN:H     | 1:44:A:PHE:HD2   | 5        | 0.13          |
| (1,2495) | 1:57:A:GLN:H     | 1:74:A:ARG:HB3   | 7        | 0.13          |
| (1,2495) | 1:57:A:GLN:H     | 1:74:A:ARG:HB2   | 14       | 0.13          |
| (1,2425) | 1:91:A:GLU:H     | 1:106:A:ALA:HB2  | 5        | 0.13          |
| (1,2392) | 1:36:A:ILE:HD13  | 1:14:A:PRO:HD3   | 2        | 0.13          |
| (1,2368) | 1:115:A:ASN:HA   | 1:75:A:PHE:HE1   | 16       | 0.13          |
| (1,2344) | 1:253:A:ILE:HA   | 1:254:A:GLU:HG2  | 2        | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2344) | 1:253:A:ILE:HA | 1:254:A:GLU:HG2 | 7        | 0.13          |
| (1,2311) | 1:58:A:VAL:H   | 1:71:A:LEU:HD22 | 2        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB2  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB2  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB2  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB2  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB3  | 3        | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB2  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB2  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB3  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB3  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB2  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB2  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3 | 1:85:A:ARG:HB3  | 10       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB2  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD2 | 1:85:A:ARG:HB3  | 18       | 0.13          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB2  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB2  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB3  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB3  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB2  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB2  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB3  | 18       | 0.13          |
| (1,2301) | 1:85:A:ARG:HD3   | 1:85:A:ARG:HB3  | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 2        | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE2 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD2  | 1:116:A:LYS:HE3 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE2 | 18       | 0.13          |
| (1,2270) | 1:116:A:LYS:HD3  | 1:116:A:LYS:HE3 | 18       | 0.13          |
| (1,2219) | 1:204:A:GLU:HA   | 1:203:A:ALA:H   | 13       | 0.13          |
| (1,2150) | 1:104:A:VAL:HG12 | 1:56:A:ILE:HG21 | 20       | 0.13          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 3        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 4        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 5        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 6        | 0.13          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 6        | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 14       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 17       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 18       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 18       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 19       | 0.13          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 19       | 0.13          |
| (1,2074) | 1:11:A:ASP:HB3  | 1:36:A:ILE:HG12 | 1        | 0.13          |
| (1,1963) | 1:80:A:ILE:HD13 | 1:77:A:LEU:HA   | 18       | 0.13          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 7        | 0.13          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 7        | 0.13          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 7        | 0.13          |
| (1,1928) | 1:44:A:PHE:HA   | 1:156:A:ASN:HB2 | 10       | 0.13          |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 5        | 0.13          |
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 5        | 0.13          |
| (1,1187) | 1:62:A:GLU:HB2  | 1:60:A:GLU:HA   | 18       | 0.13          |
| (1,1187) | 1:62:A:GLU:HB3  | 1:60:A:GLU:HA   | 18       | 0.13          |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG21 | 11       | 0.13          |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG22 | 11       | 0.13          |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG23 | 11       | 0.13          |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG21 | 19       | 0.13          |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG22 | 19       | 0.13          |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG23 | 19       | 0.13          |
| (1,841)  | 1:10:A:LEU:HA   | 1:10:A:LEU:HG   | 2        | 0.13          |
| (2,13)   | 1:20:A:GLU:H    | 1:57:A:GLN:O    | 15       | 0.12          |
| (1,3189) | 1:12:A:VAL:HG13 | 1:33:A:ASN:HA   | 7        | 0.12          |
| (1,3177) | 1:26:A:MET:HE1  | 1:29:A:LEU:H    | 19       | 0.12          |
| (1,3175) | 1:64:A:ALA:HB2  | 1:149:A:ARG:HD3 | 17       | 0.12          |
| (1,3128) | 1:141:A:TYR:HD2 | 1:144:A:GLU:HG3 | 6        | 0.12          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD11 | 1:70:A:ASN:HD22 | 13       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD12 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD13 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD21 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD22 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD21 | 13       | 0.12          |
| (1,3119) | 1:72:A:LEU:HD23 | 1:70:A:ASN:HD22 | 13       | 0.12          |
| (1,3089) | 1:35:A:THR:HB   | 1:36:A:ILE:H    | 17       | 0.12          |
| (1,3086) | 1:26:A:MET:HE2  | 1:19:A:LEU:H    | 9        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3005) | 1:159:A:GLU:H   | 1:159:A:GLU:HG2  | 7        | 0.12          |
| (1,3005) | 1:159:A:GLU:H   | 1:159:A:GLU:HG2  | 7        | 0.12          |
| (1,3005) | 1:159:A:GLU:H   | 1:159:A:GLU:HG3  | 7        | 0.12          |
| (1,3005) | 1:159:A:GLU:H   | 1:159:A:GLU:HG3  | 7        | 0.12          |
| (1,2999) | 1:140:A:LYS:H   | 1:141:A:TYR:HB2  | 13       | 0.12          |
| (1,2967) | 1:99:A:ASN:H    | 1:36:A:ILE:HD11  | 20       | 0.12          |
| (1,2935) | 1:65:A:MET:H    | 1:66:A:THR:HA    | 16       | 0.12          |
| (1,2916) | 1:96:A:ILE:H    | 1:39:A:LYS:HG3   | 20       | 0.12          |
| (1,2862) | 1:86:A:GLY:H    | 1:85:A:ARG:HB3   | 13       | 0.12          |
| (1,2831) | 1:138:A:ALA:H   | 1:137:A:GLU:HB2  | 7        | 0.12          |
| (1,2831) | 1:138:A:ALA:H   | 1:137:A:GLU:HB2  | 17       | 0.12          |
| (1,2830) | 1:138:A:ALA:H   | 1:137:A:GLU:HB2  | 7        | 0.12          |
| (1,2830) | 1:138:A:ALA:H   | 1:137:A:GLU:HB2  | 17       | 0.12          |
| (1,2820) | 1:136:A:GLN:H   | 1:135:A:VAL:HG13 | 8        | 0.12          |
| (1,2820) | 1:136:A:GLN:H   | 1:135:A:VAL:HG12 | 19       | 0.12          |
| (1,2809) | 1:132:A:GLU:H   | 1:131:A:ILE:HG23 | 8        | 0.12          |
| (1,2726) | 1:38:A:THR:H    | 1:30:A:ILE:HD13  | 12       | 0.12          |
| (1,2696) | 1:127:A:SER:H   | 1:127:A:SER:HA   | 14       | 0.12          |
| (1,2696) | 1:127:A:SER:H   | 1:127:A:SER:HA   | 17       | 0.12          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB2   | 5        | 0.12          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB1   | 8        | 0.12          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB1   | 14       | 0.12          |
| (1,2613) | 1:9:A:LEU:HA    | 1:9:A:LEU:H      | 14       | 0.12          |
| (1,2595) | 1:64:A:ALA:H    | 1:63:A:ARG:HA    | 4        | 0.12          |
| (1,2541) | 1:55:A:LEU:H    | 1:54:A:VAL:HG21  | 18       | 0.12          |
| (1,2429) | 1:27:A:THR:H    | 1:26:A:MET:HE3   | 13       | 0.12          |
| (1,2425) | 1:91:A:GLU:H    | 1:106:A:ALA:HB1  | 19       | 0.12          |
| (1,2392) | 1:36:A:ILE:HD13 | 1:14:A:PRO:HD3   | 10       | 0.12          |
| (1,2256) | 1:94:A:PHE:HE2  | 1:19:A:LEU:HB2   | 14       | 0.12          |
| (1,2216) | 1:13:A:ALA:HB1  | 1:32:A:ARG:HB2   | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG11  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG11  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG12  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG12  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG13  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG13  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG21  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG21  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG22  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG22  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG23  | 14       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG23  | 14       | 0.12          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 15       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 16       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 17       | 0.12          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 17       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 1        | 0.12          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 1        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 2        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 7        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 8        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 8        | 0.12          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 9        | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 10       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG21 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG22 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG23 | 11       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG11 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG12 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB | 1:12:A:VAL:HG13 | 12       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 12       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 13       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 16       | 0.12          |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 16       | 0.12          |
| (1,2009) | 1:9:A:LEU:HA    | 1:9:A:LEU:H     | 14       | 0.12          |
| (1,2004) | 1:98:A:ALA:HA   | 1:100:A:GLY:HA2 | 14       | 0.12          |
| (1,1967) | 1:80:A:ILE:HD11 | 1:54:A:VAL:HA   | 1        | 0.12          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 6        | 0.12          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 6        | 0.12          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 6        | 0.12          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 13       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 13       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 13       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 17       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 17       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 17       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 18       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 18       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 18       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 20       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 20       | 0.12          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 20       | 0.12          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2 | 4        | 0.12          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB3 | 4        | 0.12          |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 2        | 0.12          |
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 2        | 0.12          |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 18       | 0.12          |
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 18       | 0.12          |
| (1,1443) | 1:80:A:ILE:HB   | 1:80:A:ILE:H    | 9        | 0.12          |
| (1,1106) | 1:35:A:THR:HG21 | 1:34:A:SER:HA   | 19       | 0.12          |
| (1,1106) | 1:35:A:THR:HG22 | 1:34:A:SER:HA   | 19       | 0.12          |
| (1,1106) | 1:35:A:THR:HG23 | 1:34:A:SER:HA   | 19       | 0.12          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG21 | 9        | 0.12          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG22 | 9        | 0.12          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG23 | 9        | 0.12          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG21 | 9        | 0.12          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG22 | 9        | 0.12          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG23 | 9        | 0.12          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG21 | 18       | 0.12          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG22 | 18       | 0.12          |
| (1,942)  | 1:37:A:PRO:HB2  | 1:38:A:THR:HG23 | 18       | 0.12          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG21 | 18       | 0.12          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG22 | 18       | 0.12          |
| (1,942)  | 1:37:A:PRO:HB3  | 1:38:A:THR:HG23 | 18       | 0.12          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG21 | 14       | 0.12          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG22 | 14       | 0.12          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG23 | 14       | 0.12          |
| (1,760)  | 1:65:A:MET:HA   | 1:66:A:THR:HG21 | 15       | 0.12          |
| (1,760)  | 1:65:A:MET:HA   | 1:66:A:THR:HG22 | 15       | 0.12          |
| (1,760)  | 1:65:A:MET:HA   | 1:66:A:THR:HG23 | 15       | 0.12          |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB2  | 2        | 0.12          |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB3  | 2        | 0.12          |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB2  | 8        | 0.12          |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB3  | 8        | 0.12          |
| (1,285)  | 1:85:A:ARG:HG2  | 1:47:A:TYR:HA   | 9        | 0.12          |
| (1,285)  | 1:85:A:ARG:HG3  | 1:47:A:TYR:HA   | 9        | 0.12          |
| (1,3180) | 1:35:A:THR:HA   | 1:36:A:ILE:HG12 | 2        | 0.11          |
| (1,3174) | 1:70:A:ASN:HD21 | 1:15:A:LEU:HB2  | 15       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3159) | 1:15:A:LEU:HD12 | 1:136:A:GLN:H    | 18       | 0.11          |
| (1,3151) | 1:13:A:ALA:HA   | 1:96:A:ILE:HG22  | 17       | 0.11          |
| (1,3135) | 1:83:A:ALA:H    | 1:82:A:PRO:HB2   | 4        | 0.11          |
| (1,3026) | 1:141:A:TYR:H   | 1:140:A:LYS:HD2  | 12       | 0.11          |
| (1,2947) | 1:69:A:ASN:H    | 1:69:A:ASN:HD21  | 14       | 0.11          |
| (1,2924) | 1:54:A:VAL:H    | 1:77:A:LEU:HD22  | 11       | 0.11          |
| (1,2866) | 1:12:A:VAL:H    | 1:11:A:ASP:H     | 16       | 0.11          |
| (1,2824) | 1:146:A:GLU:H   | 1:143:A:ALA:HA   | 1        | 0.11          |
| (1,2824) | 1:146:A:GLU:H   | 1:143:A:ALA:HA   | 13       | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG11 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG11 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG12 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG12 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG13 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG13 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG21 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG21 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG22 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG22 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG23 | 4        | 0.11          |
| (1,2745) | 1:135:A:VAL:H   | 1:135:A:VAL:HG23 | 4        | 0.11          |
| (1,2716) | 1:19:A:LEU:H    | 1:28:A:ALA:HB2   | 19       | 0.11          |
| (1,2649) | 1:100:A:GLY:H   | 1:98:A:ALA:HB3   | 18       | 0.11          |
| (1,2598) | 1:142:A:LYS:H   | 1:142:A:LYS:HD2  | 10       | 0.11          |
| (1,2530) | 1:90:A:ILE:H    | 1:43:A:ILE:HG21  | 8        | 0.11          |
| (1,2501) | 1:31:A:LYS:H    | 1:28:A:ALA:HB2   | 9        | 0.11          |
| (1,2463) | 1:108:A:ASP:H   | 1:77:A:LEU:HG    | 8        | 0.11          |
| (1,2425) | 1:91:A:GLU:H    | 1:106:A:ALA:HB3  | 8        | 0.11          |
| (1,2420) | 1:119:A:ILE:H   | 1:101:A:ILE:HG23 | 13       | 0.11          |
| (1,2412) | 1:102:A:LEU:H   | 1:118:A:THR:HG21 | 9        | 0.11          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD11 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 17       | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD12 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD13 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD21 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD22 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB2   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2284) | 1:55:A:LEU:HD23 | 1:74:A:ARG:HB3   | 17       | 0.11          |
| (1,2219) | 1:204:A:GLU:HA  | 1:203:A:ALA:H    | 12       | 0.11          |
| (1,2169) | 1:56:A:ILE:HG22 | 1:58:A:VAL:HB    | 11       | 0.11          |
| (1,2144) | 1:27:A:THR:HG21 | 1:156:A:ASN:HD22 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG11  | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG11  | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB   | 1:25:A:VAL:HG12  | 1        | 0.11          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 1        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 2        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 3        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 4        | 0.11          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 4        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 5        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 6        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 7        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 8        | 0.11          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 8        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 9        | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 10       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 11       | 0.11          |

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| Key      | Atom-1        | Atom-2          | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 11       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 12       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 13       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG13 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG21 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG22 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG23 | 18       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG11 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB | 1:25:A:VAL:HG12 | 19       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG12 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG13 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG13 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG21 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG21 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG22 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG22 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG23 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG23 | 19       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG11 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG11 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG12 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG12 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG13 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG13 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG21 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG21 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG22 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG22 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG23 | 20       | 0.11          |
| (1,2084) | 1:25:A:VAL:HB  | 1:25:A:VAL:HG23 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG11 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG11 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG12 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG12 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG13 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG13 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG21 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG21 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG22 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG22 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG23 | 20       | 0.11          |
| (1,2079) | 1:12:A:VAL:HB  | 1:12:A:VAL:HG23 | 20       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD11 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD11 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD12 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD12 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD13 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD13 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD21 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD21 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD22 | 12       | 0.11          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD22 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD23 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD2 | 1:55:A:LEU:HD23 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD11 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD11 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD12 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD12 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD13 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD13 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD21 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD21 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD22 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD22 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD23 | 12       | 0.11          |
| (1,2064) | 1:74:A:ARG:HD3 | 1:55:A:LEU:HD23 | 12       | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD11 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD11 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD12 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD12 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD13 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD13 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD21 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD21 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD22 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD22 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD23 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB2 | 1:17:A:LEU:HD23 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD11 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD11 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD12 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD12 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD13 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD13 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD21 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD21 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD22 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD22 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD23 | 8        | 0.11          |
| (1,2062) | 1:17:A:LEU:HB3 | 1:17:A:LEU:HD23 | 8        | 0.11          |
| (1,2058) | 1:220:A:ASN:HA | 1:221:A:PRO:HD2 | 7        | 0.11          |
| (1,2058) | 1:220:A:ASN:HA | 1:221:A:PRO:HD2 | 7        | 0.11          |
| (1,2058) | 1:220:A:ASN:HA | 1:221:A:PRO:HD3 | 7        | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2058) | 1:220:A:ASN:HA  | 1:221:A:PRO:HD3 | 7        | 0.11          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 1        | 0.11          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 1        | 0.11          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 1        | 0.11          |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 19       | 0.11          |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 19       | 0.11          |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 19       | 0.11          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB2 | 12       | 0.11          |
| (1,1920) | 1:21:A:THR:H    | 1:158:A:LEU:HB3 | 12       | 0.11          |
| (1,1785) | 1:67:A:LYS:HA   | 1:69:A:ASN:H    | 2        | 0.11          |
| (1,1752) | 1:22:A:ALA:HB1  | 1:47:A:TYR:H    | 13       | 0.11          |
| (1,1752) | 1:22:A:ALA:HB2  | 1:47:A:TYR:H    | 13       | 0.11          |
| (1,1752) | 1:22:A:ALA:HB3  | 1:47:A:TYR:H    | 13       | 0.11          |
| (1,1752) | 1:22:A:ALA:HB1  | 1:47:A:TYR:H    | 16       | 0.11          |
| (1,1752) | 1:22:A:ALA:HB2  | 1:47:A:TYR:H    | 16       | 0.11          |
| (1,1752) | 1:22:A:ALA:HB3  | 1:47:A:TYR:H    | 16       | 0.11          |
| (1,1720) | 1:61:A:GLY:H    | 1:18:A:GLY:H    | 17       | 0.11          |
| (1,1698) | 1:11:A:ASP:HA   | 1:12:A:VAL:H    | 5        | 0.11          |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 7        | 0.11          |
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 7        | 0.11          |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 9        | 0.11          |
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 9        | 0.11          |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 14       | 0.11          |
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 14       | 0.11          |
| (1,1621) | 1:67:A:LYS:HG2  | 1:68:A:ASP:H    | 8        | 0.11          |
| (1,1621) | 1:67:A:LYS:HG3  | 1:68:A:ASP:H    | 8        | 0.11          |
| (1,1621) | 1:67:A:LYS:HG2  | 1:68:A:ASP:H    | 19       | 0.11          |
| (1,1621) | 1:67:A:LYS:HG3  | 1:68:A:ASP:H    | 19       | 0.11          |
| (1,1607) | 1:12:A:VAL:H    | 1:11:A:ASP:H    | 16       | 0.11          |
| (1,1187) | 1:62:A:GLU:HB2  | 1:60:A:GLU:HA   | 1        | 0.11          |
| (1,1187) | 1:62:A:GLU:HB3  | 1:60:A:GLU:HA   | 1        | 0.11          |
| (1,1187) | 1:62:A:GLU:HB2  | 1:60:A:GLU:HA   | 13       | 0.11          |
| (1,1187) | 1:62:A:GLU:HB3  | 1:60:A:GLU:HA   | 13       | 0.11          |
| (1,1106) | 1:35:A:THR:HG21 | 1:34:A:SER:HA   | 5        | 0.11          |
| (1,1106) | 1:35:A:THR:HG22 | 1:34:A:SER:HA   | 5        | 0.11          |
| (1,1106) | 1:35:A:THR:HG23 | 1:34:A:SER:HA   | 5        | 0.11          |
| (1,1106) | 1:35:A:THR:HG21 | 1:34:A:SER:HA   | 14       | 0.11          |
| (1,1106) | 1:35:A:THR:HG22 | 1:34:A:SER:HA   | 14       | 0.11          |
| (1,1106) | 1:35:A:THR:HG23 | 1:34:A:SER:HA   | 14       | 0.11          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG21 | 2        | 0.11          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG22 | 2        | 0.11          |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG23 | 2        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,938)  | 1:95:A:ASP:HA    | 1:38:A:THR:HG21  | 17       | 0.11          |
| (1,938)  | 1:95:A:ASP:HA    | 1:38:A:THR:HG22  | 17       | 0.11          |
| (1,938)  | 1:95:A:ASP:HA    | 1:38:A:THR:HG23  | 17       | 0.11          |
| (1,760)  | 1:65:A:MET:HA    | 1:66:A:THR:HG21  | 19       | 0.11          |
| (1,760)  | 1:65:A:MET:HA    | 1:66:A:THR:HG22  | 19       | 0.11          |
| (1,760)  | 1:65:A:MET:HA    | 1:66:A:THR:HG23  | 19       | 0.11          |
| (1,520)  | 1:120:A:THR:HA   | 1:99:A:ASN:HB2   | 1        | 0.11          |
| (1,520)  | 1:120:A:THR:HA   | 1:99:A:ASN:HB3   | 1        | 0.11          |
| (1,290)  | 1:152:A:VAL:HG11 | 1:150:A:GLU:HA   | 18       | 0.11          |
| (1,290)  | 1:152:A:VAL:HG12 | 1:150:A:GLU:HA   | 18       | 0.11          |
| (1,290)  | 1:152:A:VAL:HG13 | 1:150:A:GLU:HA   | 18       | 0.11          |
| (1,290)  | 1:152:A:VAL:HG21 | 1:150:A:GLU:HA   | 18       | 0.11          |
| (1,290)  | 1:152:A:VAL:HG22 | 1:150:A:GLU:HA   | 18       | 0.11          |
| (1,290)  | 1:152:A:VAL:HG23 | 1:150:A:GLU:HA   | 18       | 0.11          |
| (1,190)  | 1:142:A:LYS:HG2  | 1:139:A:GLU:HA   | 1        | 0.11          |
| (1,190)  | 1:142:A:LYS:HG3  | 1:139:A:GLU:HA   | 1        | 0.11          |
| (1,190)  | 1:142:A:LYS:HG2  | 1:139:A:GLU:HA   | 13       | 0.11          |
| (1,190)  | 1:142:A:LYS:HG3  | 1:139:A:GLU:HA   | 13       | 0.11          |
| (1,3180) | 1:35:A:THR:HA    | 1:36:A:ILE:HG12  | 15       | 0.1           |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 18       | 0.1           |
| (1,3179) | 1:35:A:THR:HB    | 1:36:A:ILE:HG12  | 20       | 0.1           |
| (1,3173) | 1:70:A:ASN:HD22  | 1:126:A:LEU:HB2  | 12       | 0.1           |
| (1,3117) | 1:126:A:LEU:HB2  | 1:70:A:ASN:HD22  | 12       | 0.1           |
| (1,3107) | 1:74:A:ARG:HG3   | 1:75:A:PHE:H     | 3        | 0.1           |
| (1,3065) | 1:92:A:VAL:HG13  | 1:93:A:THR:H     | 11       | 0.1           |
| (1,3053) | 1:149:A:ARG:HB2  | 1:26:A:MET:H     | 16       | 0.1           |
| (1,3053) | 1:102:A:LEU:HB3  | 1:104:A:VAL:H    | 20       | 0.1           |
| (1,2808) | 1:132:A:GLU:H    | 1:132:A:GLU:HB3  | 11       | 0.1           |
| (1,2805) | 1:132:A:GLU:H    | 1:129:A:GLU:HA   | 3        | 0.1           |
| (1,2638) | 1:60:A:GLU:H     | 1:58:A:VAL:HG11  | 3        | 0.1           |
| (1,2622) | 1:33:A:ASN:H     | 1:13:A:ALA:HB3   | 5        | 0.1           |
| (1,2541) | 1:55:A:LEU:H     | 1:54:A:VAL:HG21  | 15       | 0.1           |
| (1,2530) | 1:90:A:ILE:H     | 1:43:A:ILE:HG21  | 17       | 0.1           |
| (1,2447) | 1:97:A:ASP:H     | 1:101:A:ILE:HD11 | 9        | 0.1           |
| (1,2256) | 1:94:A:PHE:HE2   | 1:19:A:LEU:HB2   | 2        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG11  | 1:84:A:PRO:HD2   | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG11  | 1:84:A:PRO:HD2   | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG11  | 1:84:A:PRO:HD3   | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG11  | 1:84:A:PRO:HD3   | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG11  | 1:84:A:PRO:HD2   | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG11  | 1:84:A:PRO:HD2   | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG11  | 1:84:A:PRO:HD3   | 4        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2250) | 1:87:A:VAL:HG11 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG12 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG13 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG21 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG22 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD2  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2250) | 1:87:A:VAL:HG23 | 1:84:A:PRO:HD3  | 4        | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 15       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG11 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG12 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG13 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG21 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG22 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 15       | 0.1           |
| (1,2079) | 1:12:A:VAL:HB   | 1:12:A:VAL:HG23 | 15       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD11 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD11 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD12 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD12 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD13 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD13 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD21 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD21 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD22 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD22 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD23 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB2  | 1:17:A:LEU:HD23 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD11 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD12 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD13 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD21 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD21 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD22 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD22 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD23 | 17       | 0.1           |
| (1,2062) | 1:17:A:LEU:HB3  | 1:17:A:LEU:HD23 | 17       | 0.1           |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 11       | 0.1           |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 11       | 0.1           |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 11       | 0.1           |
| (1,1933) | 1:64:A:ALA:HB1  | 1:145:A:ASP:HB2 | 16       | 0.1           |
| (1,1933) | 1:64:A:ALA:HB2  | 1:145:A:ASP:HB2 | 16       | 0.1           |
| (1,1933) | 1:64:A:ALA:HB3  | 1:145:A:ASP:HB2 | 16       | 0.1           |
| (1,1673) | 1:116:A:LYS:HB2 | 1:116:A:LYS:H   | 1        | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1673) | 1:116:A:LYS:HB3 | 1:116:A:LYS:H   | 1        | 0.1           |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG21 | 16       | 0.1           |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG22 | 16       | 0.1           |
| (1,938)  | 1:95:A:ASP:HA   | 1:38:A:THR:HG23 | 16       | 0.1           |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG21 | 12       | 0.1           |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG22 | 12       | 0.1           |
| (1,937)  | 1:39:A:LYS:HA   | 1:38:A:THR:HG23 | 12       | 0.1           |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB2  | 5        | 0.1           |
| (1,520)  | 1:120:A:THR:HA  | 1:99:A:ASN:HB3  | 5        | 0.1           |
| (1,504)  | 1:39:A:LYS:HB2  | 1:39:A:LYS:HE2  | 17       | 0.1           |
| (1,504)  | 1:39:A:LYS:HB2  | 1:39:A:LYS:HE3  | 17       | 0.1           |
| (1,504)  | 1:39:A:LYS:HB3  | 1:39:A:LYS:HE2  | 17       | 0.1           |
| (1,504)  | 1:39:A:LYS:HB3  | 1:39:A:LYS:HE3  | 17       | 0.1           |



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

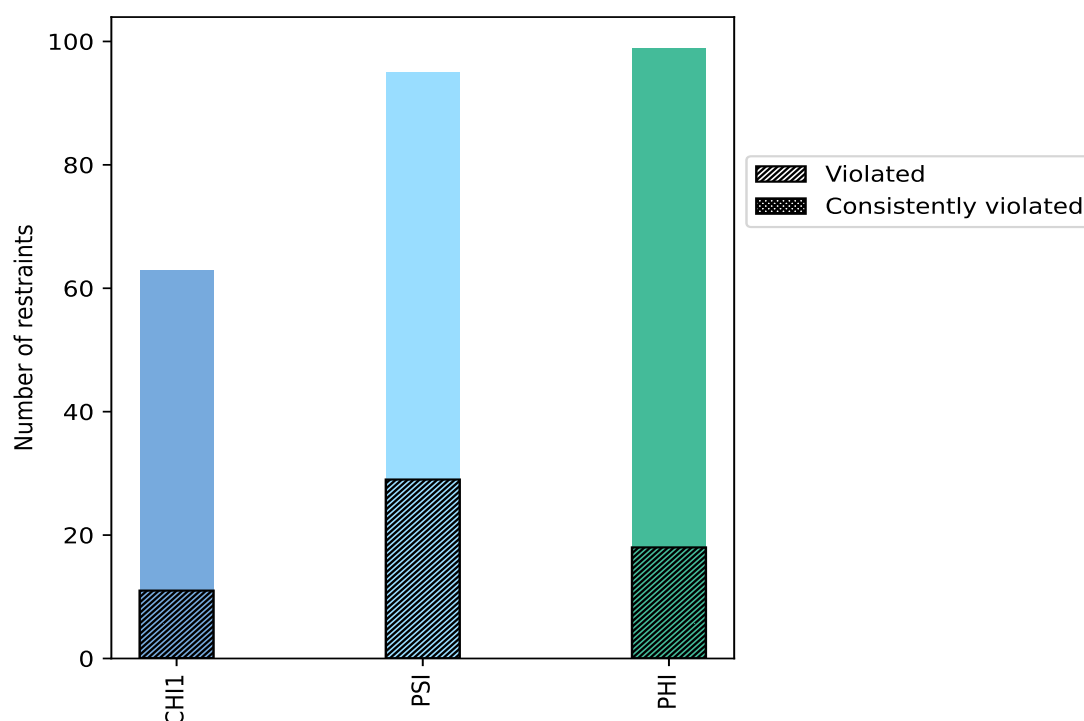
### 10.1 Summary of dihedral-angle violations [i](#)

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       | 63    | 24.5           | 11                    | 17.5           | 4.3            | 0                                  | 0.0            | 0.0            |
| PSI        | 95    | 37.0           | 29                    | 30.5           | 11.3           | 0                                  | 0.0            | 0.0            |
| PHI        | 99    | 38.5           | 18                    | 18.2           | 7.0            | 0                                  | 0.0            | 0.0            |
| Total      | 257   | 100.0          | 58                    | 22.6           | 22.6           | 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](#)



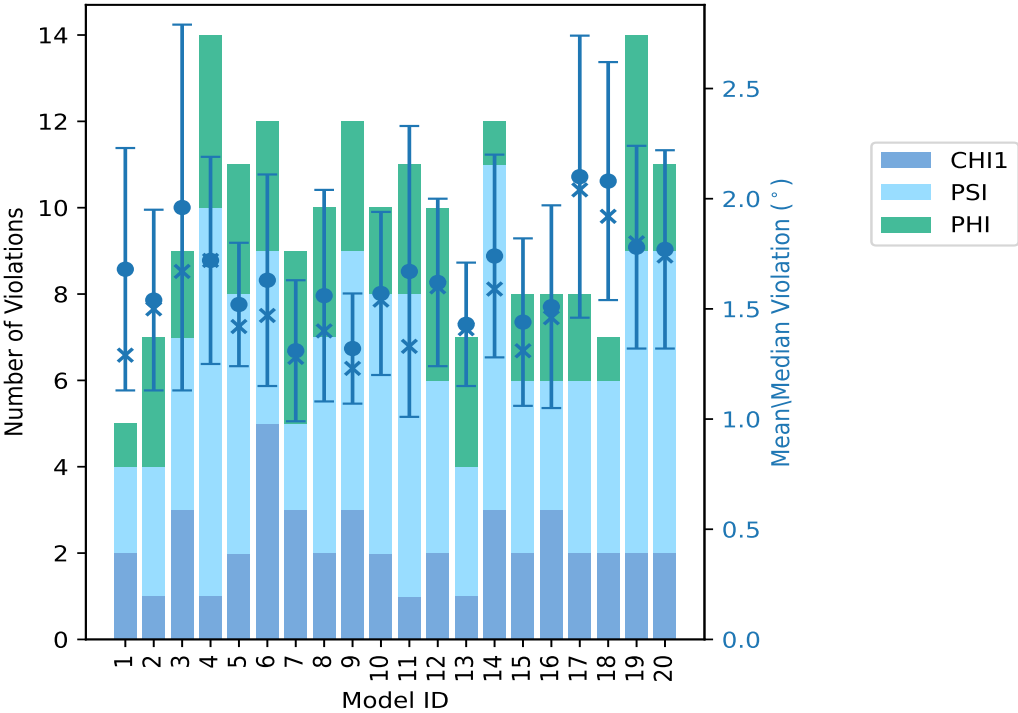
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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                 | PSI | PHI | Total |          |         |        |            |
| 1        | 2                    | 2   | 1   | 5     | 1.68     | 2.56    | 0.55   | 1.29       |
| 2        | 1                    | 3   | 3   | 7     | 1.54     | 2.21    | 0.41   | 1.5        |
| 3        | 3                    | 4   | 2   | 9     | 1.96     | 3.68    | 0.83   | 1.67       |
| 4        | 1                    | 9   | 4   | 14    | 1.72     | 2.87    | 0.47   | 1.72       |
| 5        | 2                    | 6   | 3   | 11    | 1.52     | 2.1     | 0.28   | 1.42       |
| 6        | 5                    | 4   | 3   | 12    | 1.63     | 2.53    | 0.48   | 1.47       |
| 7        | 3                    | 2   | 4   | 9     | 1.31     | 2.09    | 0.32   | 1.28       |
| 8        | 2                    | 5   | 3   | 10    | 1.56     | 2.67    | 0.48   | 1.4        |
| 9        | 3                    | 6   | 3   | 12    | 1.32     | 1.84    | 0.25   | 1.23       |
| 10       | 2                    | 6   | 2   | 10    | 1.57     | 2.34    | 0.37   | 1.54       |
| 11       | 1                    | 7   | 3   | 11    | 1.67     | 3.06    | 0.66   | 1.33       |
| 12       | 2                    | 4   | 4   | 10    | 1.62     | 2.18    | 0.38   | 1.6        |
| 13       | 1                    | 3   | 3   | 7     | 1.43     | 2.03    | 0.28   | 1.41       |
| 14       | 3                    | 8   | 1   | 12    | 1.74     | 2.57    | 0.46   | 1.59       |
| 15       | 2                    | 4   | 2   | 8     | 1.44     | 2.43    | 0.38   | 1.31       |
| 16       | 3                    | 3   | 2   | 8     | 1.51     | 2.57    | 0.46   | 1.46       |
| 17       | 2                    | 4   | 2   | 8     | 2.1      | 3.57    | 0.64   | 2.04       |
| 18       | 2                    | 4   | 1   | 7     | 2.08     | 2.95    | 0.54   | 1.92       |
| 19       | 2                    | 7   | 5   | 14    | 1.78     | 2.91    | 0.46   | 1.8        |
| 20       | 2                    | 7   | 2   | 11    | 1.77     | 2.43    | 0.45   | 1.74       |

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                          | PSI | PHI | Total | Count <sup>1</sup>       | %    |
| 6                             | 10  | 6   | 22    | 1                        | 5.0  |
| 2                             | 4   | 6   | 12    | 2                        | 10.0 |
| 0                             | 6   | 2   | 8     | 3                        | 15.0 |
| 0                             | 2   | 3   | 5     | 4                        | 20.0 |
| 1                             | 2   | 0   | 3     | 5                        | 25.0 |
| 0                             | 1   | 0   | 1     | 6                        | 30.0 |
| 0                             | 2   | 0   | 2     | 7                        | 35.0 |
| 0                             | 0   | 0   | 0     | 8                        | 40.0 |
| 0                             | 0   | 0   | 0     | 9                        | 45.0 |
| 0                             | 1   | 0   | 1     | 10                       | 50.0 |
| 0                             | 0   | 0   | 0     | 11                       | 55.0 |

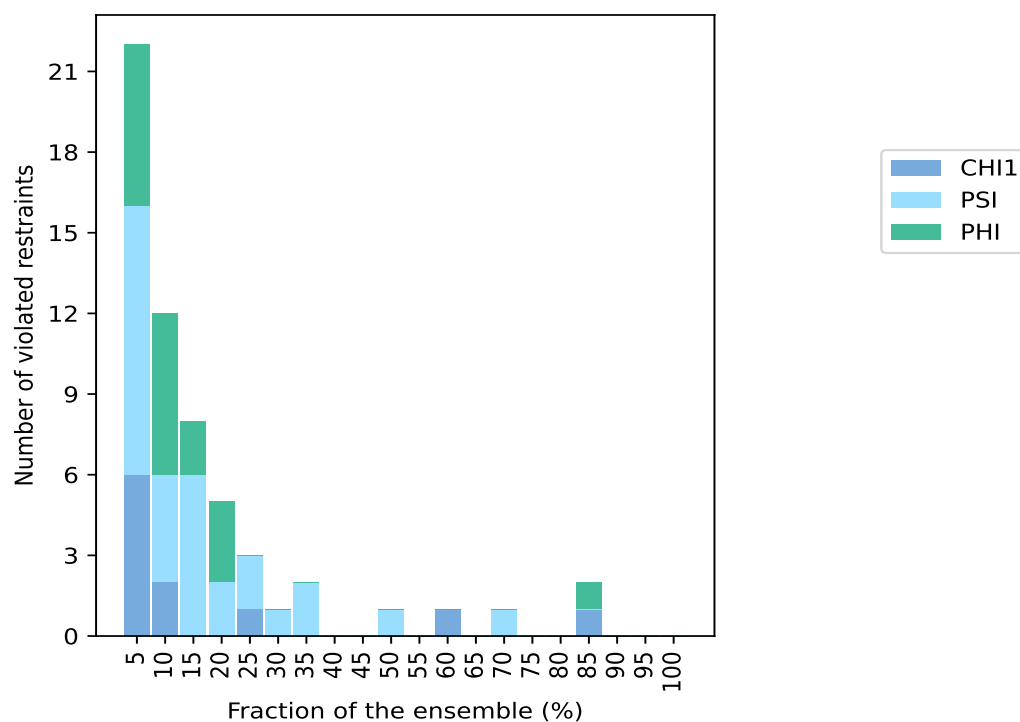
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| Number of violated restraints |     |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-----|-------|--------------------------|-------|
| CHI1                          | PSI | PHI | Total | Count <sup>1</sup>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

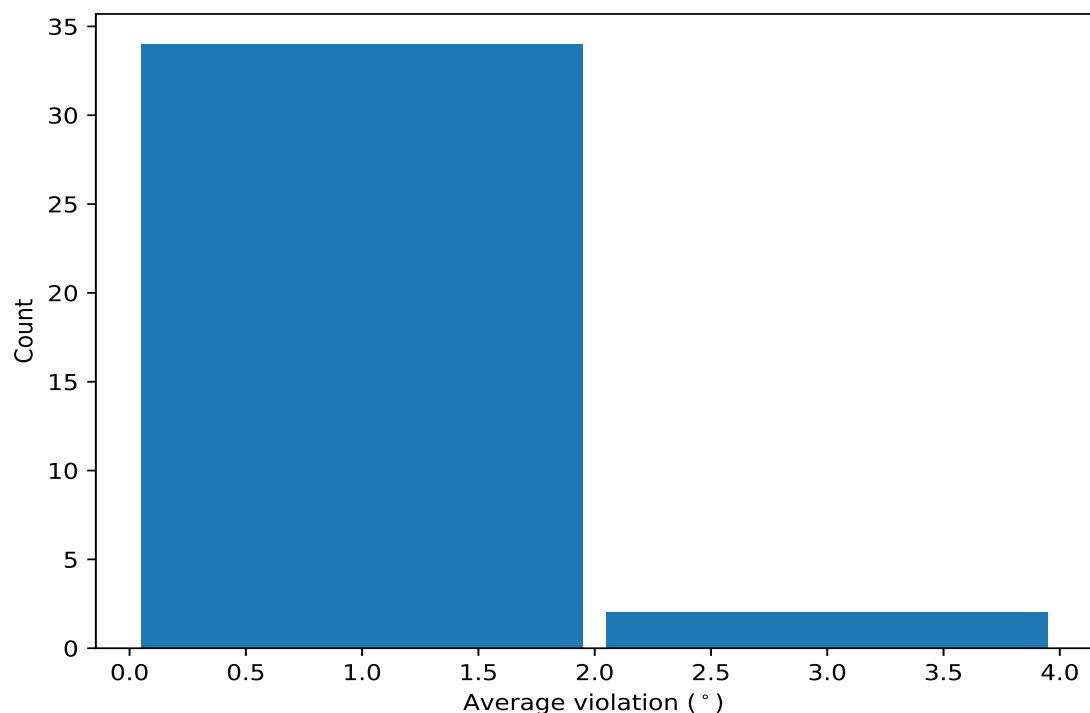


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|----------------|---------------------|------|-----------------|--------|
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 17                  | 2.06 | 0.51            | 2.13   |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 17                  | 1.8  | 0.55            | 1.66   |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 14                  | 1.96 | 0.61            | 1.82   |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 12                  | 1.71 | 0.38            | 1.76   |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N   | 10                  | 1.65 | 0.71            | 1.42   |
| (1,108) | 1:99:A:ASN:N  | 1:99:A:ASN:CA  | 1:99:A:ASN:C   | 1:100:A:GLY:N  | 7                   | 1.61 | 0.6             | 1.42   |
| (1,80)  | 1:77:A:LEU:N  | 1:77:A:LEU:CA  | 1:77:A:LEU:C   | 1:78:A:SER:N   | 7                   | 1.53 | 0.36            | 1.35   |
| (1,192) | 1:158:A:LEU:N | 1:158:A:LEU:CA | 1:158:A:LEU:C  | 1:159:A:GLU:N  | 6                   | 1.67 | 0.25            | 1.69   |
| (1,203) | 1:47:A:TYR:N  | 1:47:A:TYR:CA  | 1:47:A:TYR:CB  | 1:47:A:TYR:CG  | 5                   | 1.76 | 0.64            | 1.4    |
| (1,29)  | 1:39:A:LYS:N  | 1:39:A:LYS:CA  | 1:39:A:LYS:C   | 1:40:A:GLN:N   | 5                   | 1.76 | 0.24            | 1.9    |
| (1,138) | 1:118:A:THR:N | 1:118:A:THR:CA | 1:118:A:THR:C  | 1:119:A:ILE:N  | 5                   | 1.38 | 0.23            | 1.4    |
| (1,65)  | 1:63:A:ARG:C  | 1:64:A:ALA:N   | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 4                   | 2.08 | 0.55            | 2.06   |
| (1,66)  | 1:64:A:ALA:N  | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 1:65:A:MET:N   | 4                   | 1.77 | 0.65            | 1.58   |
| (1,67)  | 1:69:A:ASN:C  | 1:70:A:ASN:N   | 1:70:A:ASN:CA  | 1:70:A:ASN:C   | 4                   | 1.64 | 0.56            | 1.58   |
| (1,163) | 1:138:A:ALA:C | 1:139:A:GLU:N  | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 4                   | 1.48 | 0.41            | 1.28   |
| (1,19)  | 1:27:A:THR:N  | 1:27:A:THR:CA  | 1:27:A:THR:C   | 1:28:A:ALA:N   | 4                   | 1.46 | 0.11            | 1.46   |
| (1,174) | 1:144:A:GLU:N | 1:144:A:GLU:CA | 1:144:A:GLU:C  | 1:145:A:ASP:N  | 3                   | 1.82 | 0.41            | 2.0    |
| (1,43)  | 1:46:A:THR:N  | 1:46:A:THR:CA  | 1:46:A:THR:C   | 1:47:A:TYR:N   | 3                   | 1.7  | 0.22            | 1.69   |
| (1,194) | 1:159:A:GLU:N | 1:159:A:GLU:CA | 1:159:A:GLU:C  | 1:160:A:SER:N  | 3                   | 1.67 | 0.42            | 1.88   |
| (1,11)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:THR:N   | 3                   | 1.48 | 0.03            | 1.46   |

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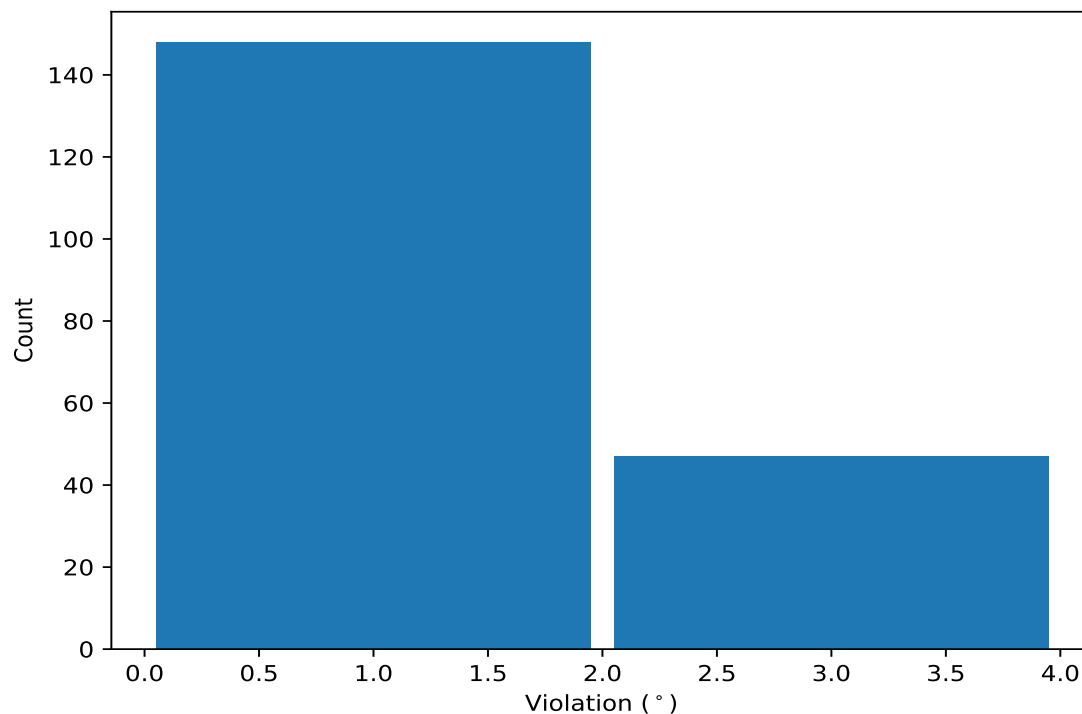
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|-----------------|---------------------|------|-----------------|--------|
| (1,21)  | 1:29:A:LEU:N  | 1:29:A:LEU:CA  | 1:29:A:LEU:C   | 1:30:A:ILE:N    | 3                   | 1.29 | 0.12            | 1.35   |
| (1,118) | 1:104:A:VAL:N | 1:104:A:VAL:CA | 1:104:A:VAL:C  | 1:105:A:THR:N   | 3                   | 1.28 | 0.08            | 1.26   |
| (1,91)  | 1:90:A:ILE:C  | 1:91:A:GLU:N   | 1:91:A:GLU:CA  | 1:91:A:GLU:C    | 3                   | 1.25 | 0.03            | 1.24   |
| (1,85)  | 1:82:A:PRO:C  | 1:83:A:ALA:N   | 1:83:A:ALA:CA  | 1:83:A:ALA:C    | 3                   | 1.13 | 0.08            | 1.13   |
| (1,189) | 1:156:A:ASN:C | 1:157:A:ALA:N  | 1:157:A:ALA:CA | 1:157:A:ALA:C   | 2                   | 1.86 | 0.33            | 1.86   |
| (1,49)  | 1:51:A:GLN:N  | 1:51:A:GLN:CA  | 1:51:A:GLN:C   | 1:52:A:PRO:N    | 2                   | 1.67 | 0.53            | 1.67   |
| (1,205) | 1:55:A:LEU:N  | 1:55:A:LEU:CA  | 1:55:A:LEU:CB  | 1:55:A:LEU:CG   | 2                   | 1.61 | 0.48            | 1.61   |
| (1,10)  | 1:19:A:LEU:C  | 1:20:A:GLU:N   | 1:20:A:GLU:CA  | 1:20:A:GLU:C    | 2                   | 1.55 | 0.14            | 1.55   |
| (1,191) | 1:157:A:ALA:C | 1:158:A:LEU:N  | 1:158:A:LEU:CA | 1:158:A:LEU:C   | 2                   | 1.48 | 0.38            | 1.48   |
| (1,165) | 1:139:A:GLU:C | 1:140:A:LYS:N  | 1:140:A:LYS:CA | 1:140:A:LYS:C   | 2                   | 1.48 | 0.02            | 1.48   |
| (1,180) | 1:147:A:VAL:N | 1:147:A:VAL:CA | 1:147:A:VAL:C  | 1:148:A:GLN:N   | 2                   | 1.38 | 0.17            | 1.38   |
| (1,142) | 1:120:A:THR:N | 1:120:A:THR:CA | 1:120:A:THR:C  | 1:121:A:ASN:N   | 2                   | 1.38 | 0.14            | 1.38   |
| (1,64)  | 1:61:A:GLY:C  | 1:62:A:GLU:N   | 1:62:A:GLU:CA  | 1:62:A:GLU:C    | 2                   | 1.33 | 0.19            | 1.33   |
| (1,51)  | 1:54:A:VAL:N  | 1:54:A:VAL:CA  | 1:54:A:VAL:C   | 1:55:A:LEU:N    | 2                   | 1.2  | 0.15            | 1.2    |
| (1,253) | 1:111:A:THR:N | 1:111:A:THR:CA | 1:111:A:THR:CB | 1:111:A:THR:OG1 | 2                   | 1.14 | 0.06            | 1.14   |
| (1,131) | 1:114:A:ALA:C | 1:115:A:ASN:N  | 1:115:A:ASN:CA | 1:115:A:ASN:C   | 2                   | 1.1  | 0.07            | 1.1    |

<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 (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 3        | 3.68          |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N   | 17       | 3.57          |
| (1,108) | 1:99:A:ASN:N  | 1:99:A:ASN:CA  | 1:99:A:ASN:C   | 1:100:A:GLY:N  | 11       | 3.06          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 18       | 2.95          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 19       | 2.91          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 3        | 2.88          |
| (1,65)  | 1:63:A:ARG:C  | 1:64:A:ALA:N   | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 4        | 2.87          |
| (1,66)  | 1:64:A:ALA:N  | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 1:65:A:MET:N   | 11       | 2.83          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 8        | 2.67          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 18       | 2.62          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 16       | 2.57          |
| (1,203) | 1:47:A:TYR:N  | 1:47:A:TYR:CA  | 1:47:A:TYR:CB  | 1:47:A:TYR:CG  | 14       | 2.57          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 1        | 2.56          |
| (1,250) | 1:66:A:THR:N  | 1:66:A:THR:CA  | 1:66:A:THR:CB  | 1:66:A:THR:OG1 | 6        | 2.53          |
| (1,203) | 1:47:A:TYR:N  | 1:47:A:TYR:CA  | 1:47:A:TYR:CB  | 1:47:A:TYR:CG  | 3        | 2.51          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 20       | 2.43          |
| (1,5)   | 1:15:A:LEU:N  | 1:15:A:LEU:CA  | 1:15:A:LEU:C   | 1:16:A:SER:N   | 15       | 2.43          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 6        | 2.4           |
| (1,67)  | 1:69:A:ASN:C  | 1:70:A:ASN:N   | 1:70:A:ASN:CA  | 1:70:A:ASN:C   | 20       | 2.36          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 17       | 2.36          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 10       | 2.34          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 14       | 2.29          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 14       | 2.23          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 20       | 2.23          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 17       | 2.21          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 2        | 2.21          |
| (1,174) | 1:144:A:GLU:N | 1:144:A:GLU:CA | 1:144:A:GLU:C  | 1:145:A:ASP:N  | 18       | 2.2           |
| (1,49)  | 1:51:A:GLN:N  | 1:51:A:GLN:CA  | 1:51:A:GLN:C   | 1:52:A:PRO:N   | 8        | 2.2           |
| (1,189) | 1:156:A:ASN:C | 1:157:A:ALA:N  | 1:157:A:ALA:CA | 1:157:A:ALA:C  | 19       | 2.19          |
| (1,163) | 1:138:A:ALA:C | 1:139:A:GLU:N  | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 12       | 2.18          |
| (1,65)  | 1:63:A:ARG:C  | 1:64:A:ALA:N   | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 6        | 2.18          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 4        | 2.15          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 4        | 2.14          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 12       | 2.13          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 20       | 2.13          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 1        | 2.1           |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 5        | 2.1           |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 19       | 2.09          |
| (1,205) | 1:55:A:LEU:N  | 1:55:A:LEU:CA  | 1:55:A:LEU:CB  | 1:55:A:LEU:CG  | 17       | 2.09          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 7        | 2.09          |
| (1,194) | 1:159:A:GLU:N | 1:159:A:GLU:CA | 1:159:A:GLU:C  | 1:160:A:SER:N  | 10       | 2.04          |
| (1,192) | 1:158:A:LEU:N | 1:158:A:LEU:CA | 1:158:A:LEU:C  | 1:159:A:GLU:N  | 14       | 2.04          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 13       | 2.03          |
| (1,80)  | 1:77:A:LEU:N  | 1:77:A:LEU:CA  | 1:77:A:LEU:C   | 1:78:A:SER:N   | 4        | 2.01          |
| (1,80)  | 1:77:A:LEU:N  | 1:77:A:LEU:CA  | 1:77:A:LEU:C   | 1:78:A:SER:N   | 14       | 2.01          |
| (1,76)  | 1:75:A:PHE:N  | 1:75:A:PHE:CA  | 1:75:A:PHE:C   | 1:76:A:GLU:N   | 12       | 2.01          |
| (1,174) | 1:144:A:GLU:N | 1:144:A:GLU:CA | 1:144:A:GLU:C  | 1:145:A:ASP:N  | 19       | 2.0           |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,67)  | 1:69:A:ASN:C  | 1:70:A:ASN:N   | 1:70:A:ASN:CA  | 1:70:A:ASN:C   | 5        | 1.99          |
| (1,43)  | 1:46:A:THR:N  | 1:46:A:THR:CA  | 1:46:A:THR:C   | 1:47:A:TYR:N   | 19       | 1.98          |
| (1,29)  | 1:39:A:LYS:N  | 1:39:A:LYS:CA  | 1:39:A:LYS:C   | 1:40:A:GLN:N   | 17       | 1.98          |
| (1,29)  | 1:39:A:LYS:N  | 1:39:A:LYS:CA  | 1:39:A:LYS:C   | 1:40:A:GLN:N   | 19       | 1.97          |
| (1,65)  | 1:63:A:ARG:C  | 1:64:A:ALA:N   | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 19       | 1.94          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 18       | 1.92          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 11       | 1.91          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 11       | 1.91          |
| (1,29)  | 1:39:A:LYS:N  | 1:39:A:LYS:CA  | 1:39:A:LYS:C   | 1:40:A:GLN:N   | 20       | 1.9           |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N   | 2        | 1.89          |
| (1,194) | 1:159:A:GLU:N | 1:159:A:GLU:CA | 1:159:A:GLU:C  | 1:160:A:SER:N  | 4        | 1.88          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 18       | 1.88          |
| (1,192) | 1:158:A:LEU:N | 1:158:A:LEU:CA | 1:158:A:LEU:C  | 1:159:A:GLU:N  | 18       | 1.87          |
| (1,191) | 1:157:A:ALA:C | 1:158:A:LEU:N  | 1:158:A:LEU:CA | 1:158:A:LEU:C  | 4        | 1.87          |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N   | 4        | 1.86          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 6        | 1.84          |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N   | 9        | 1.84          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 12       | 1.8           |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 2        | 1.77          |
| (1,80)  | 1:77:A:LEU:N  | 1:77:A:LEU:CA  | 1:77:A:LEU:C   | 1:78:A:SER:N   | 20       | 1.74          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 3        | 1.73          |
| (1,192) | 1:158:A:LEU:N | 1:158:A:LEU:CA | 1:158:A:LEU:C  | 1:159:A:GLU:N  | 17       | 1.72          |
| (1,138) | 1:118:A:THR:N | 1:118:A:THR:CA | 1:118:A:THR:C  | 1:119:A:ILE:N  | 9        | 1.72          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 16       | 1.71          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 10       | 1.7           |
| (1,43)  | 1:46:A:THR:N  | 1:46:A:THR:CA  | 1:46:A:THR:C   | 1:47:A:TYR:N   | 5        | 1.69          |
| (1,10)  | 1:19:A:LEU:C  | 1:20:A:GLU:N   | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 10       | 1.69          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 12       | 1.68          |
| (1,37)  | 1:43:A:ILE:N  | 1:43:A:ILE:CA  | 1:43:A:ILE:C   | 1:44:A:PHE:N   | 14       | 1.68          |
| (1,192) | 1:158:A:LEU:N | 1:158:A:LEU:CA | 1:158:A:LEU:C  | 1:159:A:GLU:N  | 3        | 1.67          |
| (1,66)  | 1:64:A:ALA:N  | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 1:65:A:MET:N   | 19       | 1.67          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 8        | 1.66          |
| (1,48)  | 1:50:A:ASN:C  | 1:51:A:GLN:N   | 1:51:A:GLN:CA  | 1:51:A:GLN:C   | 3        | 1.63          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 19       | 1.61          |
| (1,44)  | 1:46:A:THR:C  | 1:47:A:TYR:N   | 1:47:A:TYR:CA  | 1:47:A:TYR:C   | 16       | 1.59          |
| (1,29)  | 1:39:A:LYS:N  | 1:39:A:LYS:CA  | 1:39:A:LYS:C   | 1:40:A:GLN:N   | 10       | 1.59          |
| (1,19)  | 1:27:A:THR:N  | 1:27:A:THR:CA  | 1:27:A:THR:C   | 1:28:A:ALA:N   | 4        | 1.59          |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N   | 6        | 1.59          |
| (1,19)  | 1:27:A:THR:N  | 1:27:A:THR:CA  | 1:27:A:THR:C   | 1:28:A:ALA:N   | 20       | 1.56          |
| (1,180) | 1:147:A:VAL:N | 1:147:A:VAL:CA | 1:147:A:VAL:C  | 1:148:A:GLN:N  | 5        | 1.55          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 9        | 1.55          |
| (1,13)  | 1:22:A:ALA:N  | 1:22:A:ALA:CA  | 1:22:A:ALA:C   | 1:23:A:GLY:N   | 13       | 1.54          |
| (1,189) | 1:156:A:ASN:C | 1:157:A:ALA:N  | 1:157:A:ALA:CA | 1:157:A:ALA:C  | 12       | 1.53          |
| (1,142) | 1:120:A:THR:N | 1:120:A:THR:CA | 1:120:A:THR:C  | 1:121:A:ASN:N  | 16       | 1.52          |
| (1,64)  | 1:61:A:GLY:C  | 1:62:A:GLU:N   | 1:62:A:GLU:CA  | 1:62:A:GLU:C   | 19       | 1.52          |
| (1,11)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:THR:N   | 19       | 1.52          |
| (1,165) | 1:139:A:GLU:C | 1:140:A:LYS:N  | 1:140:A:LYS:CA | 1:140:A:LYS:C  | 2        | 1.5           |
| (1,66)  | 1:64:A:ALA:N  | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 1:65:A:MET:N   | 14       | 1.5           |
| (1,138) | 1:118:A:THR:N | 1:118:A:THR:CA | 1:118:A:THR:C  | 1:119:A:ILE:N  | 5        | 1.49          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 14       | 1.49          |
| (1,257) | 1:127:A:SER:N | 1:127:A:SER:CA | 1:127:A:SER:CB | 1:127:A:SER:OG | 6        | 1.48          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4         | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|----------------|----------|---------------|
| (1,108) | 1:99:A:ASN:N  | 1:99:A:ASN:CA  | 1:99:A:ASN:C   | 1:100:A:GLY:N  | 10       | 1.48          |
| (1,165) | 1:139:A:GLU:C | 1:140:A:LYS:N  | 1:140:A:LYS:CA | 1:140:A:LYS:C  | 17       | 1.47          |
| (1,249) | 1:46:A:THR:N  | 1:46:A:THR:CA  | 1:46:A:THR:CB  | 1:46:A:THR:OG1 | 7        | 1.46          |
| (1,192) | 1:158:A:LEU:N | 1:158:A:LEU:CA | 1:158:A:LEU:C  | 1:159:A:GLU:N  | 15       | 1.46          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 13       | 1.46          |
| (1,11)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:THR:N   | 6        | 1.46          |
| (1,164) | 1:139:A:GLU:N | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1:140:A:LYS:N  | 14       | 1.45          |
| (1,11)  | 1:20:A:GLU:N  | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 1:21:A:THR:N   | 20       | 1.45          |
| (1,43)  | 1:46:A:THR:N  | 1:46:A:THR:CA  | 1:46:A:THR:C   | 1:47:A:TYR:N   | 4        | 1.43          |
| (1,108) | 1:99:A:ASN:N  | 1:99:A:ASN:CA  | 1:99:A:ASN:C   | 1:100:A:GLY:N  | 5        | 1.42          |
| (1,108) | 1:99:A:ASN:N  | 1:99:A:ASN:CA  | 1:99:A:ASN:C   | 1:100:A:GLY:N  | 6        | 1.42          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 17       | 1.41          |
| (1,108) | 1:99:A:ASN:N  | 1:99:A:ASN:CA  | 1:99:A:ASN:C   | 1:100:A:GLY:N  | 8        | 1.41          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 9        | 1.41          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 13       | 1.41          |
| (1,10)  | 1:19:A:LEU:C  | 1:20:A:GLU:N   | 1:20:A:GLU:CA  | 1:20:A:GLU:C   | 4        | 1.41          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG  | 16       | 1.4           |
| (1,203) | 1:47:A:TYR:N  | 1:47:A:TYR:CA  | 1:47:A:TYR:CB  | 1:47:A:TYR:CG  | 8        | 1.4           |
| (1,138) | 1:118:A:THR:N | 1:118:A:THR:CA | 1:118:A:THR:C  | 1:119:A:ILE:N  | 19       | 1.4           |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 4        | 1.4           |
| (1,21)  | 1:29:A:LEU:N  | 1:29:A:LEU:CA  | 1:29:A:LEU:C   | 1:30:A:ILE:N   | 8        | 1.4           |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 8        | 1.39          |
| (1,118) | 1:104:A:VAL:N | 1:104:A:VAL:CA | 1:104:A:VAL:C  | 1:105:A:THR:N  | 5        | 1.38          |
| (1,29)  | 1:39:A:LYS:N  | 1:39:A:LYS:CA  | 1:39:A:LYS:C   | 1:40:A:GLN:N   | 14       | 1.38          |
| (1,108) | 1:99:A:ASN:N  | 1:99:A:ASN:CA  | 1:99:A:ASN:C   | 1:100:A:GLY:N  | 20       | 1.37          |
| (1,19)  | 1:27:A:THR:N  | 1:27:A:THR:CA  | 1:27:A:THR:C   | 1:28:A:ALA:N   | 9        | 1.37          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 7        | 1.36          |
| (1,80)  | 1:77:A:LEU:N  | 1:77:A:LEU:CA  | 1:77:A:LEU:C   | 1:78:A:SER:N   | 15       | 1.35          |
| (1,51)  | 1:54:A:VAL:N  | 1:54:A:VAL:CA  | 1:54:A:VAL:C   | 1:55:A:LEU:N   | 11       | 1.35          |
| (1,21)  | 1:29:A:LEU:N  | 1:29:A:LEU:CA  | 1:29:A:LEU:C   | 1:30:A:ILE:N   | 12       | 1.35          |
| (1,179) | 1:146:A:GLU:C | 1:147:A:VAL:N  | 1:147:A:VAL:CA | 1:147:A:VAL:C  | 15       | 1.34          |
| (1,172) | 1:143:A:ALA:N | 1:143:A:ALA:CA | 1:143:A:ALA:C  | 1:144:A:GLU:N  | 5        | 1.34          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 7        | 1.33          |
| (1,41)  | 1:45:A:THR:N  | 1:45:A:THR:CA  | 1:45:A:THR:C   | 1:46:A:THR:N   | 10       | 1.33          |
| (1,19)  | 1:27:A:THR:N  | 1:27:A:THR:CA  | 1:27:A:THR:C   | 1:28:A:ALA:N   | 11       | 1.33          |
| (1,65)  | 1:63:A:ARG:C  | 1:64:A:ALA:N   | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 11       | 1.32          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 5        | 1.31          |
| (1,91)  | 1:90:A:ILE:C  | 1:91:A:GLU:N   | 1:91:A:GLU:CA  | 1:91:A:GLU:C   | 5        | 1.3           |
| (1,163) | 1:138:A:ALA:C | 1:139:A:GLU:N  | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 1        | 1.29          |
| (1,80)  | 1:77:A:LEU:N  | 1:77:A:LEU:CA  | 1:77:A:LEU:C   | 1:78:A:SER:N   | 8        | 1.29          |
| (1,203) | 1:47:A:TYR:N  | 1:47:A:TYR:CA  | 1:47:A:TYR:CB  | 1:47:A:TYR:CG  | 7        | 1.28          |
| (1,192) | 1:158:A:LEU:N | 1:158:A:LEU:CA | 1:158:A:LEU:C  | 1:159:A:GLU:N  | 11       | 1.28          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 2        | 1.27          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG | 15       | 1.27          |
| (1,163) | 1:138:A:ALA:C | 1:139:A:GLU:N  | 1:139:A:GLU:CA | 1:139:A:GLU:C  | 6        | 1.27          |
| (1,138) | 1:118:A:THR:N | 1:118:A:THR:CA | 1:118:A:THR:C  | 1:119:A:ILE:N  | 6        | 1.27          |
| (1,118) | 1:104:A:VAL:N | 1:104:A:VAL:CA | 1:104:A:VAL:C  | 1:105:A:THR:N  | 4        | 1.26          |
| (1,174) | 1:144:A:GLU:N | 1:144:A:GLU:CA | 1:144:A:GLU:C  | 1:145:A:ASP:N  | 15       | 1.25          |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N   | 3        | 1.25          |
| (1,142) | 1:120:A:THR:N | 1:120:A:THR:CA | 1:120:A:THR:C  | 1:121:A:ASN:N  | 9        | 1.24          |
| (1,91)  | 1:90:A:ILE:C  | 1:91:A:GLU:N   | 1:91:A:GLU:CA  | 1:91:A:GLU:C   | 13       | 1.24          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4          | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|-----------------|----------|---------------|
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N    | 1        | 1.24          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG   | 15       | 1.23          |
| (1,217) | 1:108:A:ASP:N | 1:108:A:ASP:CA | 1:108:A:ASP:CB | 1:108:A:ASP:CG  | 1        | 1.23          |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG   | 3        | 1.22          |
| (1,180) | 1:147:A:VAL:N | 1:147:A:VAL:CA | 1:147:A:VAL:C  | 1:148:A:GLN:N   | 20       | 1.22          |
| (1,91)  | 1:90:A:ILE:C  | 1:91:A:GLU:N   | 1:91:A:GLU:CA  | 1:91:A:GLU:C    | 14       | 1.22          |
| (1,85)  | 1:82:A:PRO:C  | 1:83:A:ALA:N   | 1:83:A:ALA:CA  | 1:83:A:ALA:C    | 13       | 1.22          |
| (1,253) | 1:111:A:THR:N | 1:111:A:THR:CA | 1:111:A:THR:CB | 1:111:A:THR:OG1 | 9        | 1.21          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C   | 15       | 1.21          |
| (1,144) | 1:129:A:GLU:N | 1:129:A:GLU:CA | 1:129:A:GLU:C  | 1:130:A:GLU:N   | 10       | 1.2           |
| (1,118) | 1:104:A:VAL:N | 1:104:A:VAL:CA | 1:104:A:VAL:C  | 1:105:A:THR:N   | 12       | 1.19          |
| (1,80)  | 1:77:A:LEU:N  | 1:77:A:LEU:CA  | 1:77:A:LEU:C   | 1:78:A:SER:N    | 10       | 1.18          |
| (1,67)  | 1:69:A:ASN:C  | 1:70:A:ASN:N   | 1:70:A:ASN:CA  | 1:70:A:ASN:C    | 12       | 1.18          |
| (1,163) | 1:138:A:ALA:C | 1:139:A:GLU:N  | 1:139:A:GLU:CA | 1:139:A:GLU:C   | 7        | 1.17          |
| (1,131) | 1:114:A:ALA:C | 1:115:A:ASN:N  | 1:115:A:ASN:CA | 1:115:A:ASN:C   | 9        | 1.17          |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N    | 12       | 1.17          |
| (1,219) | 1:125:A:ARG:N | 1:125:A:ARG:CA | 1:125:A:ARG:CB | 1:125:A:ARG:CG  | 10       | 1.14          |
| (1,205) | 1:55:A:LEU:N  | 1:55:A:LEU:CA  | 1:55:A:LEU:CB  | 1:55:A:LEU:CG   | 5        | 1.14          |
| (1,64)  | 1:61:A:GLY:C  | 1:62:A:GLU:N   | 1:62:A:GLU:CA  | 1:62:A:GLU:C    | 11       | 1.14          |
| (1,49)  | 1:51:A:GLN:N  | 1:51:A:GLN:CA  | 1:51:A:GLN:C   | 1:52:A:PRO:N    | 19       | 1.14          |
| (1,152) | 1:133:A:ARG:N | 1:133:A:ARG:CA | 1:133:A:ARG:C  | 1:134:A:MET:N   | 18       | 1.13          |
| (1,85)  | 1:82:A:PRO:C  | 1:83:A:ALA:N   | 1:83:A:ALA:CA  | 1:83:A:ALA:C    | 9        | 1.13          |
| (1,21)  | 1:29:A:LEU:N  | 1:29:A:LEU:CA  | 1:29:A:LEU:C   | 1:30:A:ILE:N    | 13       | 1.13          |
| (1,128) | 1:109:A:LYS:N | 1:109:A:LYS:CA | 1:109:A:LYS:C  | 1:110:A:SER:N   | 3        | 1.11          |
| (1,108) | 1:99:A:ASN:N  | 1:99:A:ASN:CA  | 1:99:A:ASN:C   | 1:100:A:GLY:N   | 16       | 1.11          |
| (1,80)  | 1:77:A:LEU:N  | 1:77:A:LEU:CA  | 1:77:A:LEU:C   | 1:78:A:SER:N    | 11       | 1.11          |
| (1,210) | 1:68:A:ASP:N  | 1:68:A:ASP:CA  | 1:68:A:ASP:CB  | 1:68:A:ASP:CG   | 9        | 1.1           |
| (1,191) | 1:157:A:ALA:C | 1:158:A:LEU:N  | 1:158:A:LEU:CA | 1:158:A:LEU:C   | 8        | 1.1           |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N    | 11       | 1.1           |
| (1,255) | 1:48:A:SER:N  | 1:48:A:SER:CA  | 1:48:A:SER:CB  | 1:48:A:SER:OG   | 9        | 1.09          |
| (1,127) | 1:108:A:ASP:C | 1:109:A:LYS:N  | 1:109:A:LYS:CA | 1:109:A:LYS:C   | 16       | 1.09          |
| (1,66)  | 1:64:A:ALA:N  | 1:64:A:ALA:CA  | 1:64:A:ALA:C   | 1:65:A:MET:N    | 4        | 1.09          |
| (1,253) | 1:111:A:THR:N | 1:111:A:THR:CA | 1:111:A:THR:CB | 1:111:A:THR:OG1 | 20       | 1.08          |
| (1,194) | 1:159:A:GLU:N | 1:159:A:GLU:CA | 1:159:A:GLU:C  | 1:160:A:SER:N   | 2        | 1.08          |
| (1,184) | 1:149:A:ARG:N | 1:149:A:ARG:CA | 1:149:A:ARG:C  | 1:150:A:GLU:N   | 4        | 1.08          |
| (1,203) | 1:47:A:TYR:N  | 1:47:A:TYR:CA  | 1:47:A:TYR:CB  | 1:47:A:TYR:CG   | 16       | 1.06          |
| (1,51)  | 1:54:A:VAL:N  | 1:54:A:VAL:CA  | 1:54:A:VAL:C   | 1:55:A:LEU:N    | 9        | 1.06          |
| (1,207) | 1:62:A:GLU:N  | 1:62:A:GLU:CA  | 1:62:A:GLU:CB  | 1:62:A:GLU:CG   | 6        | 1.05          |
| (1,185) | 1:149:A:ARG:C | 1:150:A:GLU:N  | 1:150:A:GLU:CA | 1:150:A:GLU:C   | 19       | 1.04          |
| (1,62)  | 1:59:A:TYR:C  | 1:60:A:GLU:N   | 1:60:A:GLU:CA  | 1:60:A:GLU:C    | 2        | 1.04          |
| (1,138) | 1:118:A:THR:N | 1:118:A:THR:CA | 1:118:A:THR:C  | 1:119:A:ILE:N   | 14       | 1.03          |
| (1,85)  | 1:82:A:PRO:C  | 1:83:A:ALA:N   | 1:83:A:ALA:CA  | 1:83:A:ALA:C    | 8        | 1.03          |
| (1,46)  | 1:49:A:ASP:C  | 1:50:A:ASN:N   | 1:50:A:ASN:CA  | 1:50:A:ASN:C    | 6        | 1.03          |
| (1,131) | 1:114:A:ALA:C | 1:115:A:ASN:N  | 1:115:A:ASN:CA | 1:115:A:ASN:C   | 7        | 1.02          |
| (1,67)  | 1:69:A:ASN:C  | 1:70:A:ASN:N   | 1:70:A:ASN:CA  | 1:70:A:ASN:C    | 7        | 1.02          |
| (1,7)   | 1:17:A:LEU:N  | 1:17:A:LEU:CA  | 1:17:A:LEU:C   | 1:18:A:GLY:N    | 7        | 1.02          |