



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:19 PM UTC

PDB ID : 6ZV3 / pdb\_00006zv3  
BMRB ID : 34540  
Title : TFIIS N-terminal domain (TND) from human MED26  
Authors : Veverka, V.  
Deposited on : 2020-07-23

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

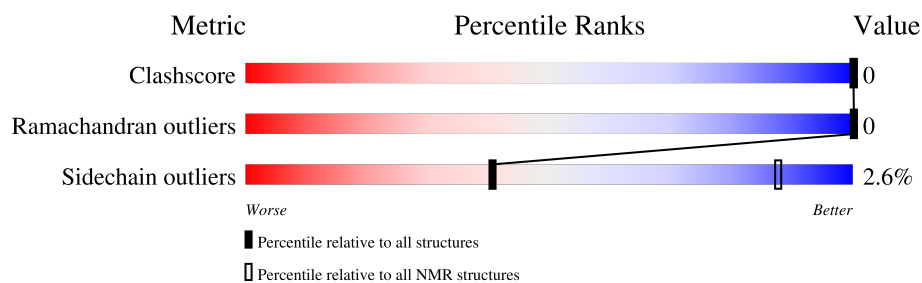
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 89%.

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     | 90     | <div> <div></div> <div>84%</div> <div></div> <div>16%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 50 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:7-A:82 (76)         | 0.32              | 18           |

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 9 clusters and 6 single-model clusters were found.

| Cluster number        | Models                                                               |
|-----------------------|----------------------------------------------------------------------|
| 1                     | 3, 8, 10, 11, 18, 19, 22, 24, 28, 30, 32, 34, 41, 44, 47, 48, 49, 50 |
| 2                     | 2, 4, 17, 21, 27, 31, 39                                             |
| 3                     | 9, 12, 15, 26, 42, 46                                                |
| 4                     | 13, 16, 36                                                           |
| 5                     | 5, 20                                                                |
| 6                     | 29, 45                                                               |
| 7                     | 14, 37                                                               |
| 8                     | 7, 38                                                                |
| 9                     | 1, 6                                                                 |
| Single-model clusters | 23; 25; 33; 35; 40; 43                                               |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1480 atoms, of which 767 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mediator of RNA polymerase II transcription subunit 26.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 90       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1480  | 446 | 767 | 131 | 134 | 2 |       |

There are 3 discrepancies between the modelled and reference sequences:

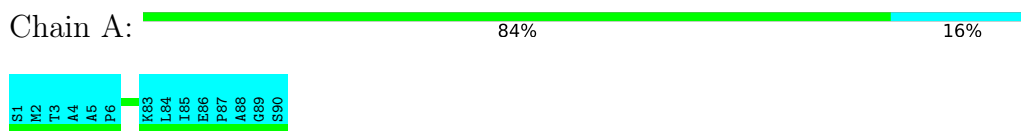
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | SER      | -      | expression tag | UNP O95402 |
| A     | 89      | GLY      | -      | expression tag | UNP O95402 |
| A     | 90      | SER      | -      | expression tag | UNP O95402 |

## 4 Residue-property plots

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

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

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26

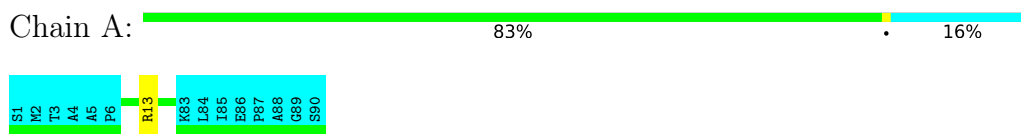


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

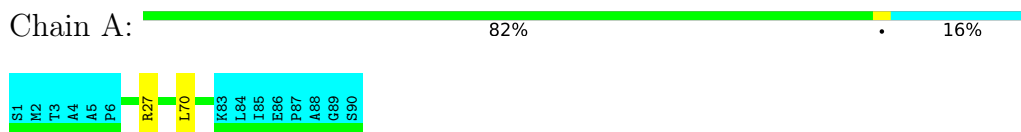
#### 4.2.1 Score per residue for model 1

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



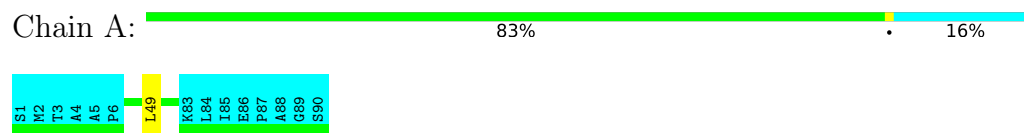
#### 4.2.2 Score per residue for model 2

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



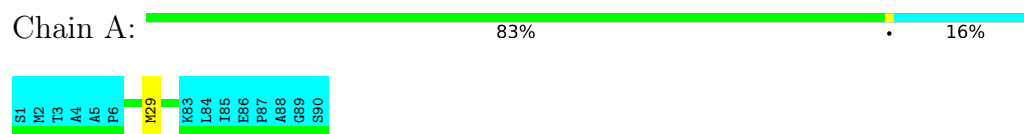
### 4.2.3 Score per residue for model 3

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



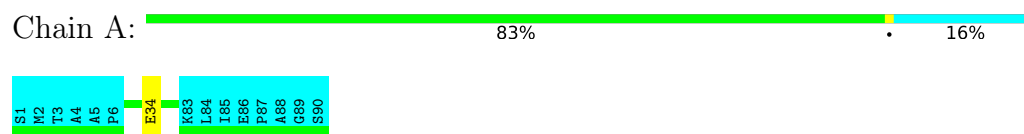
### 4.2.4 Score per residue for model 4

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



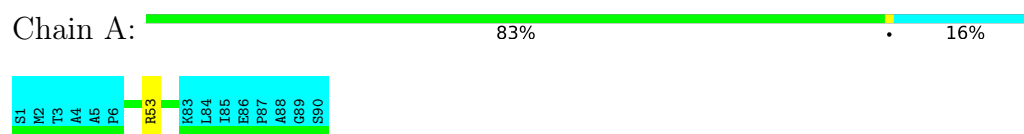
### 4.2.5 Score per residue for model 5

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



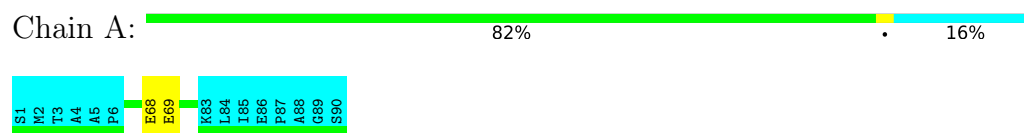
### 4.2.6 Score per residue for model 6

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



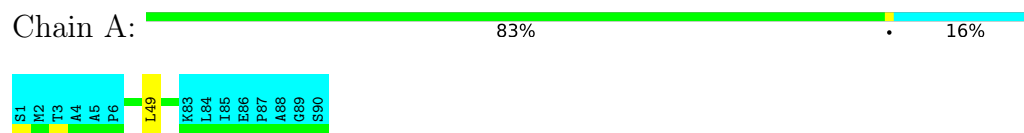
### 4.2.7 Score per residue for model 7

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



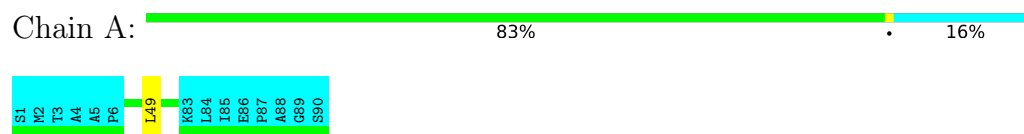
### 4.2.8 Score per residue for model 8

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



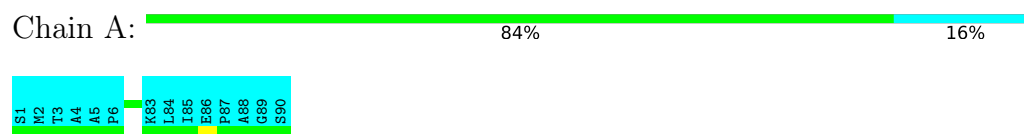
### 4.2.9 Score per residue for model 9

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



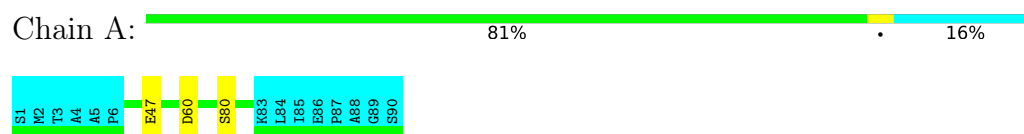
### 4.2.10 Score per residue for model 10

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



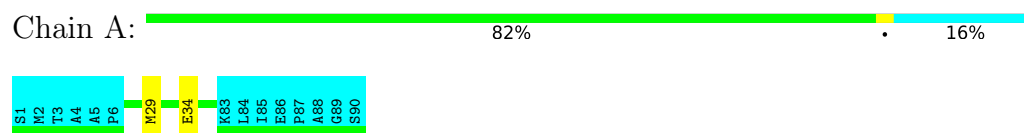
### 4.2.11 Score per residue for model 11

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



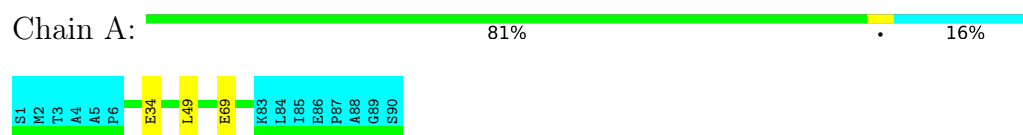
### 4.2.12 Score per residue for model 12

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



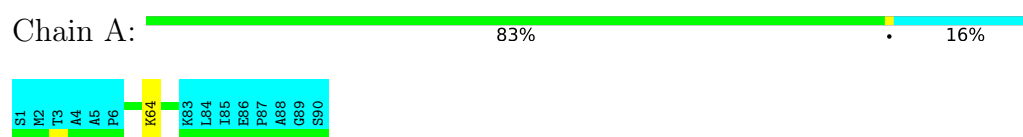
### 4.2.13 Score per residue for model 13

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



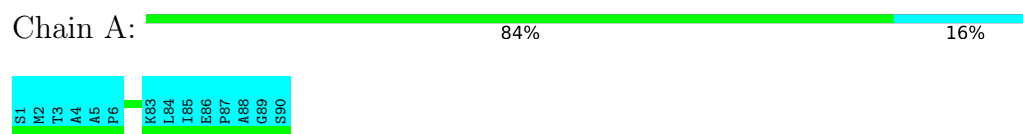
### 4.2.14 Score per residue for model 14

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



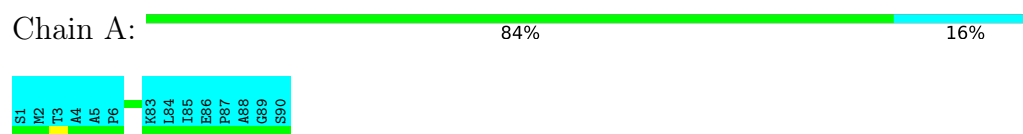
### 4.2.15 Score per residue for model 15

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



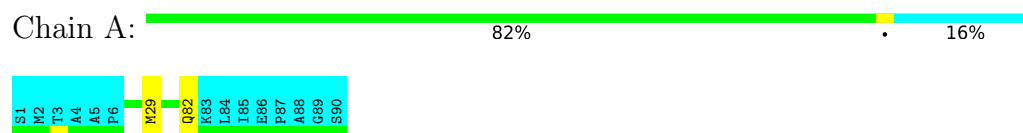
### 4.2.16 Score per residue for model 16

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



### 4.2.17 Score per residue for model 17

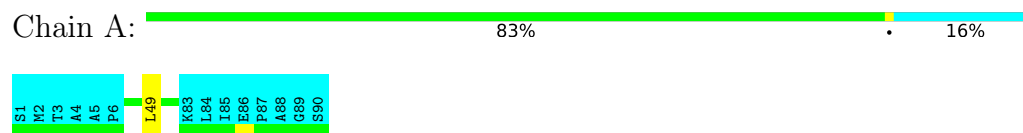
- Molecule 1: Mediator of RNA polymerase II transcription subunit 26





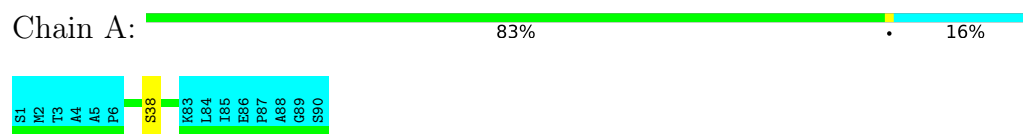
#### 4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



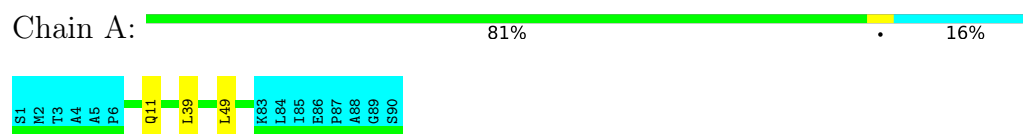
#### 4.2.19 Score per residue for model 19

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



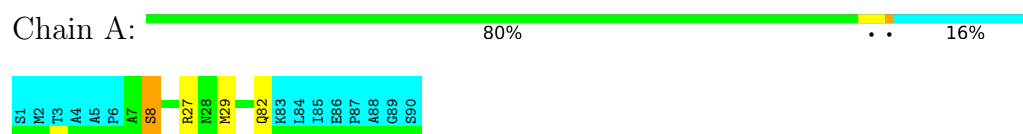
#### 4.2.20 Score per residue for model 20

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



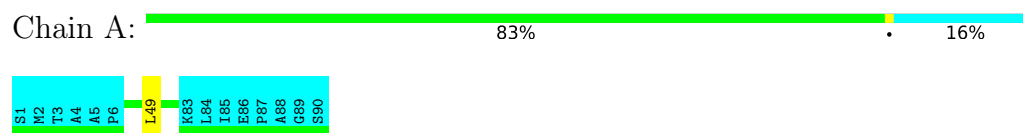
#### 4.2.21 Score per residue for model 21

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



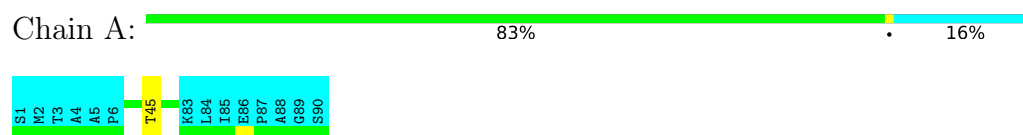
#### 4.2.22 Score per residue for model 22

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



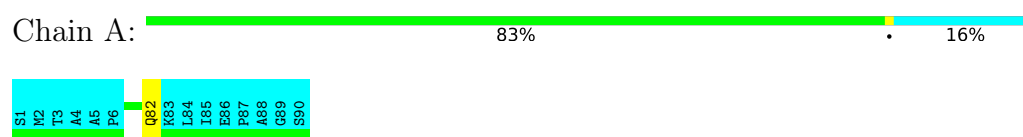
#### 4.2.23 Score per residue for model 23

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



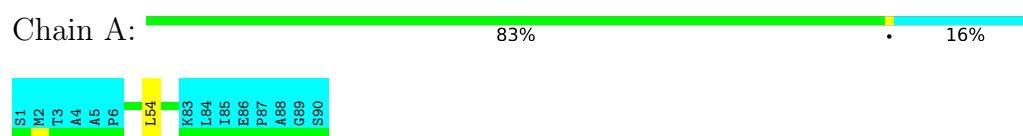
#### 4.2.24 Score per residue for model 24

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



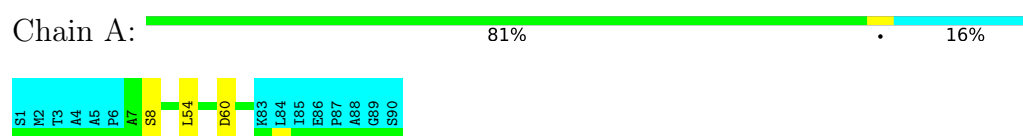
#### 4.2.25 Score per residue for model 25

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



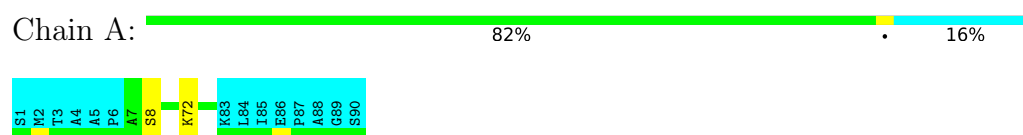
#### 4.2.26 Score per residue for model 26

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



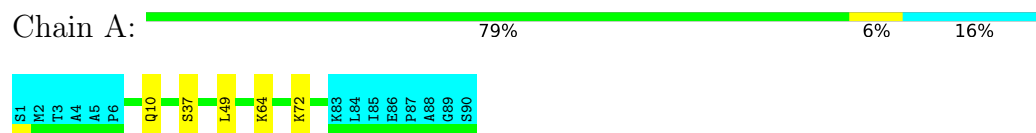
#### 4.2.27 Score per residue for model 27

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



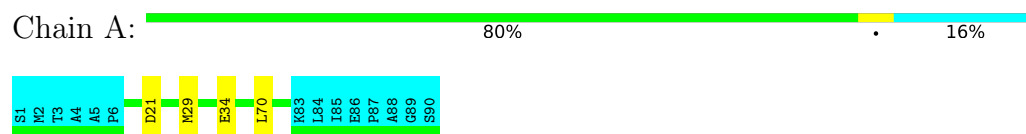
#### 4.2.28 Score per residue for model 28

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



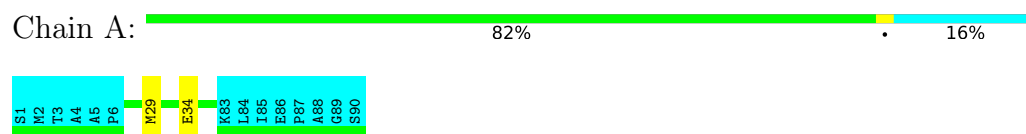
#### 4.2.29 Score per residue for model 29

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



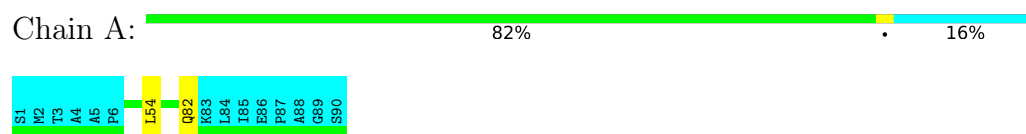
#### 4.2.30 Score per residue for model 30

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



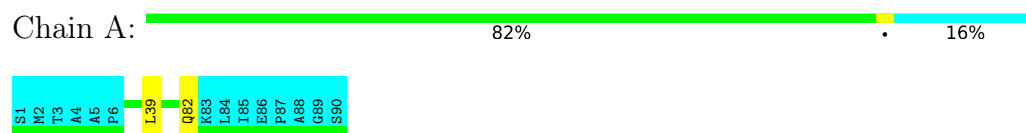
#### 4.2.31 Score per residue for model 31

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



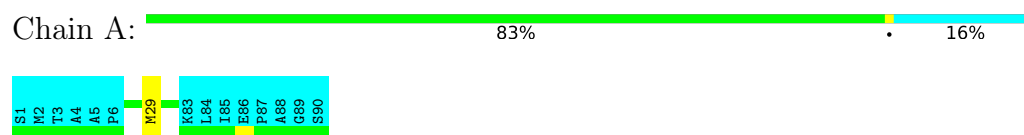
#### 4.2.32 Score per residue for model 32

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



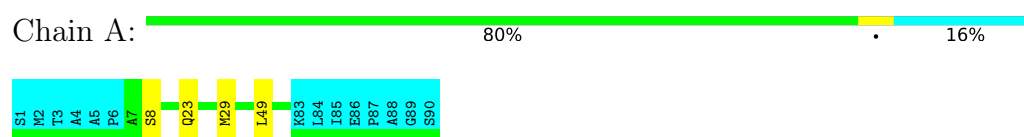
### 4.2.33 Score per residue for model 33

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



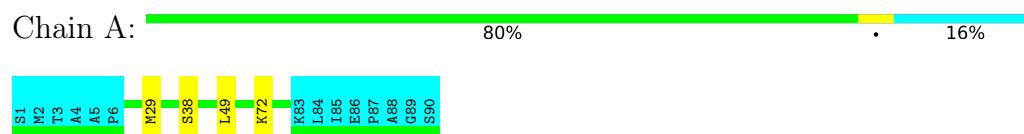
### 4.2.34 Score per residue for model 34

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



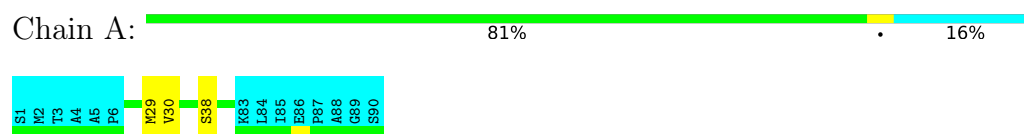
### 4.2.35 Score per residue for model 35

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



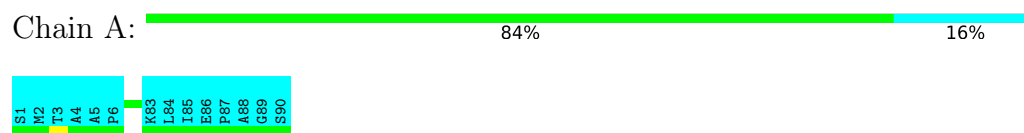
### 4.2.36 Score per residue for model 36

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



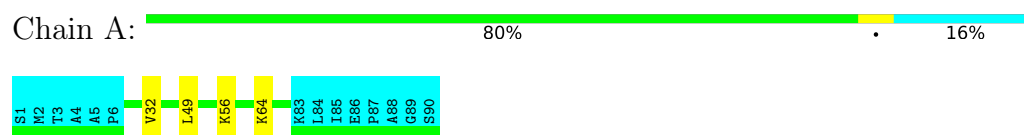
### 4.2.37 Score per residue for model 37

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



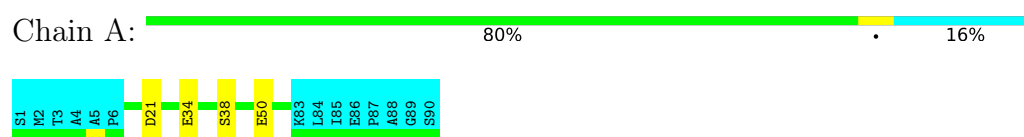
#### 4.2.38 Score per residue for model 38

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



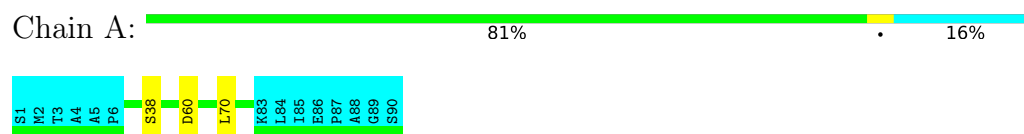
#### 4.2.39 Score per residue for model 39

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



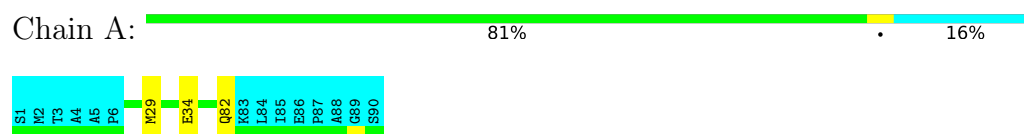
#### 4.2.40 Score per residue for model 40

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



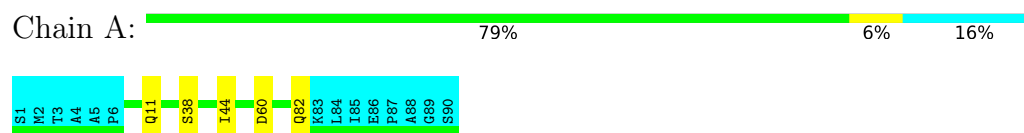
#### 4.2.41 Score per residue for model 41

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



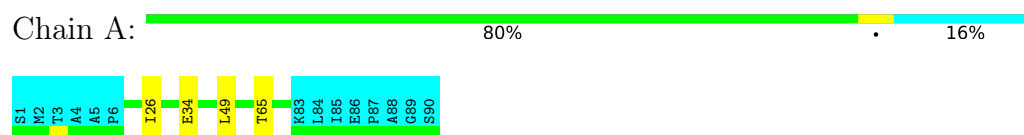
#### 4.2.42 Score per residue for model 42

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



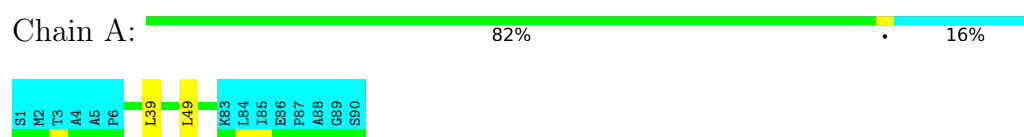
#### 4.2.43 Score per residue for model 43

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



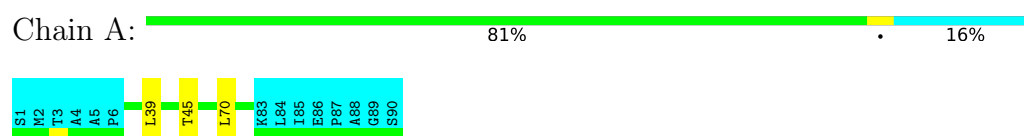
#### 4.2.44 Score per residue for model 44

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



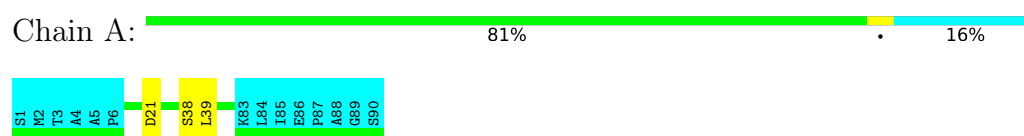
#### 4.2.45 Score per residue for model 45

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



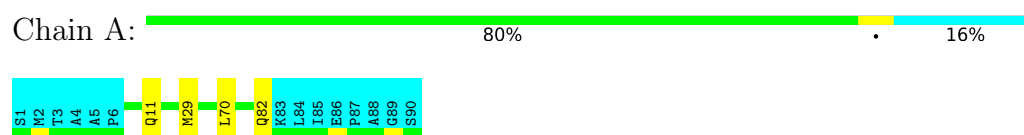
#### 4.2.46 Score per residue for model 46

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



#### 4.2.47 Score per residue for model 47

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



#### 4.2.48 Score per residue for model 48

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26

Chain A:  84% 16%



#### 4.2.49 Score per residue for model 49

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26

Chain A:  78% 6% 16%



#### 4.2.50 Score per residue for model 50

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26

Chain A:  82% 16%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, molecular dynamics*.

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CYANA         | structure calculation |         |
| YASARA        | 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                       | 1138           |
| Number of shifts mapped to atoms             | 1138           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 89%            |



## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                      | Bond angles |                      |
|-----|-------|--------------|----------------------|-------------|----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                 |
| 1   | A     | 1.00±0.17    | 0±0/624 ( 0.0± 0.1%) | 0.93±0.10   | 0±1/838 ( 0.0± 0.1%) |
| All | All   | 1.02         | 8/31200 ( 0.0%)      | 0.94        | 14/41900 ( 0.0%)     |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 26  | ILE  | CA-CB | 6.44  | 1.61        | 1.54     | 43     | 1     |
| 1   | A     | 44  | ILE  | CA-CB | 6.39  | 1.61        | 1.54     | 42     | 1     |
| 1   | A     | 30  | VAL  | CA-CB | 5.89  | 1.61        | 1.54     | 36     | 1     |
| 1   | A     | 29  | MET  | SD-CE | -5.42 | 1.66        | 1.79     | 34     | 2     |
| 1   | A     | 54  | LEU  | C-O   | -5.25 | 1.18        | 1.24     | 31     | 1     |
| 1   | A     | 66  | LYS  | C-O   | -5.18 | 1.17        | 1.24     | 49     | 1     |
| 1   | A     | 65  | THR  | CA-CB | 5.02  | 1.61        | 1.53     | 43     | 1     |

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

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 8   | SER  | CA-C-N | -6.03 | 112.65      | 119.28   | 21     | 2     |
| 1   | A     | 8   | SER  | C-N-CA | -6.03 | 112.65      | 119.28   | 21     | 2     |
| 1   | A     | 29  | MET  | N-CA-C | 5.78  | 117.58      | 111.28   | 30     | 2     |
| 1   | A     | 82  | GLN  | N-CA-C | -5.48 | 105.39      | 111.36   | 32     | 3     |
| 1   | A     | 70  | LEU  | N-CA-C | -5.26 | 105.44      | 111.07   | 45     | 3     |
| 1   | A     | 32  | VAL  | N-CA-C | -5.08 | 105.76      | 110.53   | 38     | 1     |
| 1   | A     | 21  | ASP  | N-CA-C | -5.05 | 102.82      | 110.39   | 29     | 1     |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 618   | 666      | 666      | 0±0     |
| All | All   | 30900 | 33300    | 33300    | 2       |

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 0.

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

| Atom-1       | Atom-2        | Clash(Å) | Distance(Å) | Models |       |
|--------------|---------------|----------|-------------|--------|-------|
|              |               |          |             | Worst  | Total |
| 1:A:47:GLU:H | 1:A:47:GLU:CD | 0.41     | 2.22        | 11     | 1     |
| 1:A:68:GLU:H | 1:A:68:GLU:CD | 0.41     | 2.24        | 49     | 1     |

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|---------------|------------|------------|-------------|-----|
| 1   | A     | 76/90 (84%)     | 76±0 (100±0%) | 0±0 (0±0%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 3800/4500 (84%) | 3795 (100%)   | 5 (0%)     | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |
|-----|-------|-----------------|--------------|------------|-------------|
| 1   | A     | 69/79 (87%)     | 67±1 (97±2%) | 2±1 (3±2%) | 41 88       |
| All | All   | 3450/3950 (87%) | 3360 (97%)   | 90 (3%)    | 41 88       |

All 26 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 49  | LEU  | 15             |
| 1   | A     | 34  | GLU  | 10             |
| 1   | A     | 29  | MET  | 9              |
| 1   | A     | 38  | SER  | 7              |
| 1   | A     | 82  | GLN  | 5              |
| 1   | A     | 39  | LEU  | 5              |
| 1   | A     | 60  | ASP  | 4              |
| 1   | A     | 64  | LYS  | 3              |
| 1   | A     | 11  | GLN  | 3              |
| 1   | A     | 8   | SER  | 3              |
| 1   | A     | 72  | LYS  | 3              |
| 1   | A     | 27  | ARG  | 2              |
| 1   | A     | 68  | GLU  | 2              |
| 1   | A     | 69  | GLU  | 2              |
| 1   | A     | 45  | THR  | 2              |
| 1   | A     | 54  | LEU  | 2              |
| 1   | A     | 21  | ASP  | 2              |
| 1   | A     | 50  | GLU  | 2              |
| 1   | A     | 70  | LEU  | 2              |
| 1   | A     | 13  | ARG  | 1              |
| 1   | A     | 53  | ARG  | 1              |
| 1   | A     | 80  | SER  | 1              |
| 1   | A     | 10  | GLN  | 1              |
| 1   | A     | 37  | SER  | 1              |
| 1   | A     | 23  | GLN  | 1              |
| 1   | A     | 56  | LYS  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 88% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 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                  | 1138 |
| Number of shifts mapped to atoms        | 1138 |
| 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           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 88       | $-0.39 \pm 0.16$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 86       | $0.20 \pm 0.14$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 84       | $-0.22 \pm 0.16$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 81       | $0.50 \pm 0.50$                 | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1007 atoms were assigned a chemical shift out of a possible 1126. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 371/375 (99%) | 149/150 (99%) | 150/152 (99%)   | 72/73 (99%)     |
| Sidechain | 618/730 (85%) | 424/470 (90%) | 187/221 (85%)   | 7/39 (18%)      |

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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 | 18/21 (86%)     | 10/10 (100%)         | 7/10 (70%)            | 1/1 (100%)            |
| Overall  | 1007/1126 (89%) | 583/630 (93%)        | 344/383 (90%)         | 80/113 (71%)          |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1137 atoms were assigned a chemical shift out of a possible 1291. 0 out of 15 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  | 424/442 (96%)   | 171/177 (97%)        | 172/180 (96%)         | 81/85 (95%)           |
| Sidechain | 695/828 (84%)   | 477/536 (89%)        | 211/252 (84%)         | 7/40 (18%)            |
| Aromatic  | 18/21 (86%)     | 10/10 (100%)         | 7/10 (70%)            | 1/1 (100%)            |
| Overall   | 1137/1291 (88%) | 658/723 (91%)        | 390/442 (88%)         | 89/126 (71%)          |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

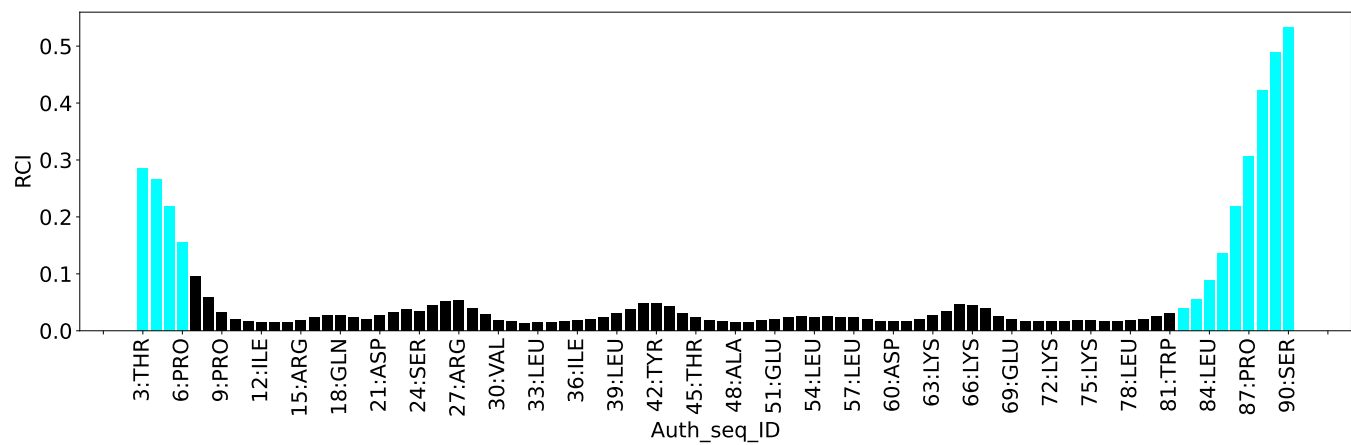
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 52  | THR  | HG1  | 4.63       | 0.08 – 2.19         | 16.6    |

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1827  |
| Intra-residue ( $ i-j =0$ )                              | 506   |
| Sequential ( $ i-j =1$ )                                 | 393   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 445   |
| Long range ( $ i-j \geq 5$ )                             | 483   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 144   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 21.9  |
| Number of long range restraints per residue <sup>1</sup> | 5.4   |

<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)  | 11.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 6.6                                    | 0.5     |
| >0.5 (Large)     | None                                   | None    |



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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 2.3                                    | 4.92    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

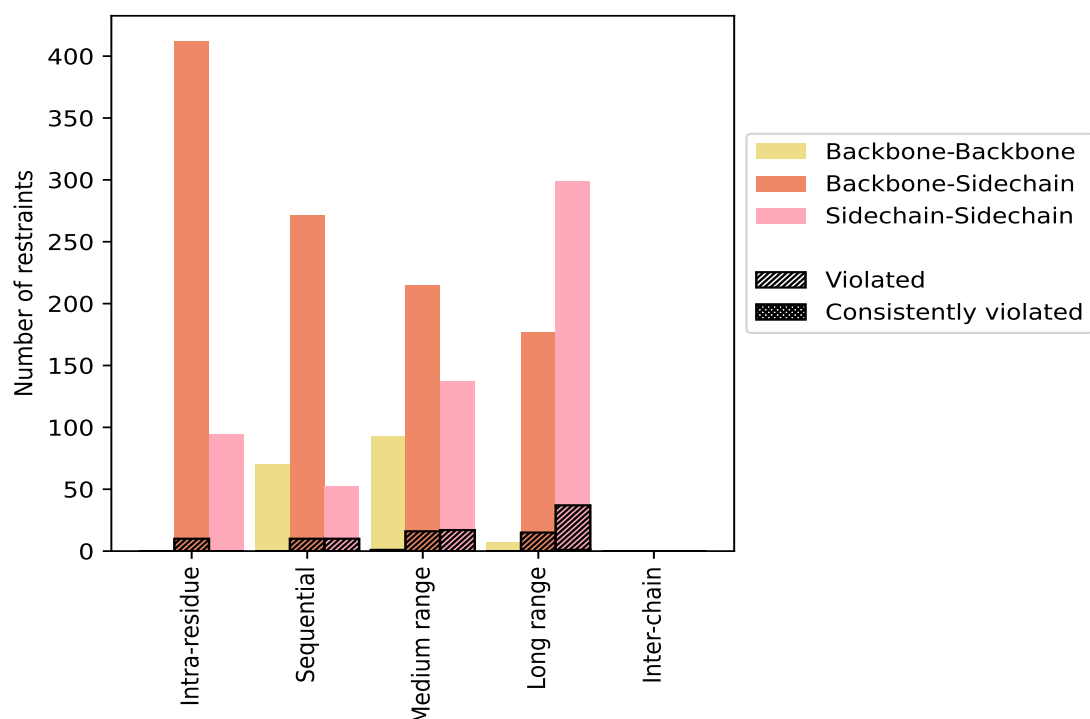
### 9.1 Summary of distance violations ⓘ

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>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">506</a>  | <a href="#">27.7</a>  | <a href="#">10</a>    | <a href="#">2.0</a>  | <a href="#">0.5</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 412                  | 22.6                  | 10                    | 2.4                  | 0.5                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 94                   | 5.1                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">393</a>  | <a href="#">21.5</a>  | <a href="#">20</a>    | <a href="#">5.1</a>  | <a href="#">1.1</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 70                   | 3.8                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 271                  | 14.8                  | 10                    | 3.7                  | 0.5                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 52                   | 2.8                   | 10                    | 19.2                 | 0.5                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">445</a>  | <a href="#">24.4</a>  | <a href="#">34</a>    | <a href="#">7.6</a>  | <a href="#">1.9</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 93                   | 5.1                   | 1                     | 1.1                  | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 215                  | 11.8                  | 16                    | 7.4                  | 0.9                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 137                  | 7.5                   | 17                    | 12.4                 | 0.9                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">483</a>  | <a href="#">26.4</a>  | <a href="#">52</a>    | <a href="#">10.8</a> | <a href="#">2.8</a> | <a href="#">1</a>                  | <a href="#">0.2</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 7                    | 0.4                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 177                  | 9.7                   | 15                    | 8.5                  | 0.8                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 299                  | 16.4                  | 37                    | 12.4                 | 2.0                 | 1                                  | 0.3                 | 0.1                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 0                    | 0.0                   | 0                     | 0.0                  | 0.0                 | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>    | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a> | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">1827</a> | <a href="#">100.0</a> | <a href="#">116</a>   | <a href="#">6.3</a>  | <a href="#">6.3</a> | <a href="#">1</a>                  | <a href="#">0.1</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 170                  | 9.3                   | 1                     | 0.6                  | 0.1                 | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 1075                 | 58.8                  | 51                    | 4.7                  | 2.8                 | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 582                  | 31.9                  | 64                    | 11.0                 | 3.5                 | 1                                  | 0.2                 | 0.1                 |

<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        | 2                    | 4               | 0               | 4               | 0               | 10    | 0.15     | 0.25    | 0.05                | 0.13       |
| 2        | 1                    | 4               | 3               | 7               | 0               | 15    | 0.18     | 0.27    | 0.05                | 0.19       |
| 3        | 0                    | 4               | 2               | 7               | 0               | 13    | 0.18     | 0.5     | 0.11                | 0.14       |
| 4        | 1                    | 3               | 2               | 6               | 0               | 12    | 0.21     | 0.32    | 0.07                | 0.22       |
| 5        | 0                    | 3               | 0               | 8               | 0               | 11    | 0.16     | 0.32    | 0.06                | 0.13       |
| 6        | 0                    | 1               | 0               | 2               | 0               | 3     | 0.14     | 0.2     | 0.04                | 0.11       |
| 7        | 0                    | 3               | 0               | 5               | 0               | 8     | 0.14     | 0.19    | 0.03                | 0.13       |
| 8        | 1                    | 4               | 3               | 9               | 0               | 17    | 0.17     | 0.26    | 0.05                | 0.17       |
| 9        | 0                    | 3               | 0               | 5               | 0               | 8     | 0.2      | 0.47    | 0.1                 | 0.16       |
| 10       | 0                    | 3               | 0               | 3               | 0               | 6     | 0.16     | 0.28    | 0.06                | 0.14       |

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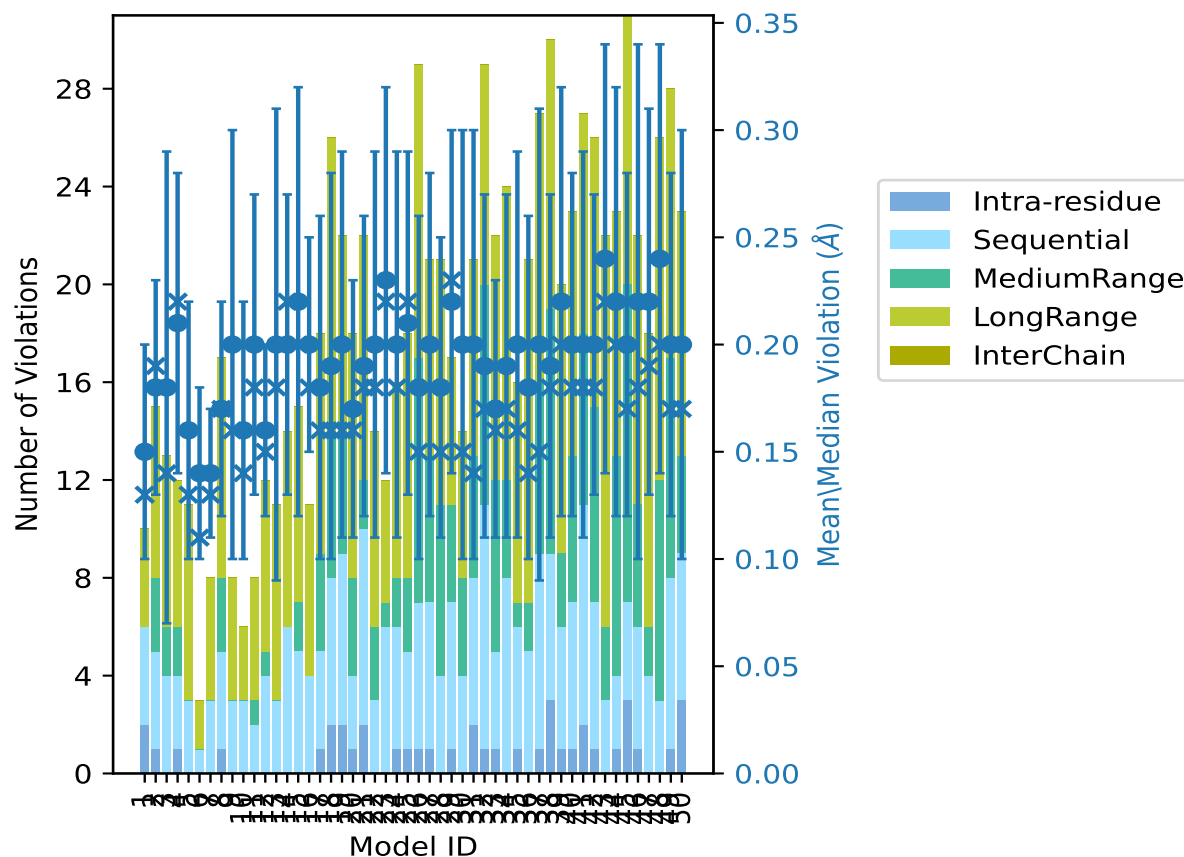
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 2               | 1               | 5               | 0               | 8     | 0.2      | 0.36    | 0.07                | 0.18       |
| 12       | 0                    | 4               | 1               | 7               | 0               | 12    | 0.16     | 0.25    | 0.04                | 0.15       |
| 13       | 0                    | 3               | 0               | 8               | 0               | 11    | 0.2      | 0.5     | 0.11                | 0.18       |
| 14       | 0                    | 6               | 0               | 8               | 0               | 14    | 0.2      | 0.31    | 0.07                | 0.22       |
| 15       | 0                    | 5               | 2               | 8               | 0               | 15    | 0.22     | 0.47    | 0.1                 | 0.2        |
| 16       | 0                    | 4               | 0               | 7               | 0               | 11    | 0.2      | 0.28    | 0.05                | 0.18       |
| 17       | 1                    | 4               | 4               | 9               | 0               | 18    | 0.18     | 0.44    | 0.08                | 0.16       |
| 18       | 2                    | 6               | 6               | 12              | 0               | 26    | 0.19     | 0.46    | 0.09                | 0.16       |
| 19       | 2                    | 7               | 5               | 8               | 0               | 22    | 0.2      | 0.46    | 0.09                | 0.16       |
| 20       | 1                    | 3               | 4               | 10              | 0               | 18    | 0.17     | 0.31    | 0.06                | 0.16       |
| 21       | 2                    | 8               | 2               | 10              | 0               | 22    | 0.19     | 0.35    | 0.07                | 0.18       |
| 22       | 0                    | 3               | 3               | 8               | 0               | 14    | 0.2      | 0.49    | 0.09                | 0.18       |
| 23       | 0                    | 6               | 1               | 5               | 0               | 12    | 0.23     | 0.39    | 0.09                | 0.22       |
| 24       | 1                    | 5               | 2               | 8               | 0               | 16    | 0.2      | 0.45    | 0.09                | 0.18       |
| 25       | 1                    | 4               | 3               | 10              | 0               | 18    | 0.21     | 0.42    | 0.08                | 0.22       |
| 26       | 1                    | 6               | 10              | 12              | 0               | 29    | 0.18     | 0.4     | 0.08                | 0.15       |
| 27       | 1                    | 6               | 6               | 8               | 0               | 21    | 0.2      | 0.37    | 0.08                | 0.18       |
| 28       | 0                    | 4               | 7               | 10              | 0               | 21    | 0.18     | 0.36    | 0.07                | 0.15       |
| 29       | 1                    | 6               | 4               | 6               | 0               | 17    | 0.22     | 0.42    | 0.08                | 0.23       |
| 30       | 0                    | 4               | 4               | 6               | 0               | 14    | 0.2      | 0.38    | 0.1                 | 0.15       |
| 31       | 2                    | 6               | 5               | 8               | 0               | 21    | 0.2      | 0.49    | 0.1                 | 0.14       |
| 32       | 1                    | 10              | 9               | 9               | 0               | 29    | 0.19     | 0.48    | 0.08                | 0.17       |
| 33       | 1                    | 4               | 7               | 10              | 0               | 22    | 0.17     | 0.29    | 0.06                | 0.16       |
| 34       | 0                    | 8               | 4               | 12              | 0               | 24    | 0.19     | 0.41    | 0.08                | 0.17       |
| 35       | 1                    | 5               | 1               | 9               | 0               | 16    | 0.2      | 0.44    | 0.09                | 0.16       |
| 36       | 0                    | 5               | 2               | 14              | 0               | 21    | 0.18     | 0.41    | 0.08                | 0.14       |
| 37       | 1                    | 8               | 7               | 11              | 0               | 27    | 0.2      | 0.44    | 0.11                | 0.15       |
| 38       | 3                    | 6               | 10              | 11              | 0               | 30    | 0.19     | 0.43    | 0.08                | 0.18       |
| 39       | 1                    | 5               | 3               | 11              | 0               | 20    | 0.22     | 0.48    | 0.1                 | 0.2        |
| 40       | 1                    | 6               | 6               | 10              | 0               | 23    | 0.2      | 0.35    | 0.08                | 0.18       |
| 41       | 2                    | 9               | 7               | 9               | 0               | 27    | 0.2      | 0.43    | 0.09                | 0.18       |
| 42       | 1                    | 6               | 8               | 11              | 0               | 26    | 0.2      | 0.42    | 0.07                | 0.18       |
| 43       | 0                    | 3               | 3               | 16              | 0               | 22    | 0.24     | 0.48    | 0.1                 | 0.22       |
| 44       | 1                    | 3               | 9               | 10              | 0               | 23    | 0.22     | 0.43    | 0.1                 | 0.2        |
| 45       | 3                    | 4               | 13              | 11              | 0               | 31    | 0.2      | 0.4     | 0.08                | 0.17       |
| 46       | 1                    | 5               | 5               | 11              | 0               | 22    | 0.22     | 0.46    | 0.12                | 0.18       |
| 47       | 0                    | 4               | 2               | 12              | 0               | 18    | 0.22     | 0.45    | 0.09                | 0.19       |
| 48       | 0                    | 3               | 9               | 14              | 0               | 26    | 0.24     | 0.46    | 0.1                 | 0.2        |
| 49       | 1                    | 7               | 9               | 11              | 0               | 28    | 0.2      | 0.38    | 0.08                | 0.17       |
| 50       | 3                    | 6               | 4               | 10              | 0               | 23    | 0.2      | 0.46    | 0.1                 | 0.17       |

<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, 1711(IR:496, SQ:373, MR:411, LR:431, 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>       | %   |
| 5                             | 5               | 12              | 13              | 0               | 35    | 1                        | 2.0 |
| 0                             | 3               | 4               | 6               | 0               | 13    | 2                        | 4.0 |
| 1                             | 0               | 3               | 8               | 0               | 12    | 3                        | 6.0 |
| 1                             | 0               | 2               | 2               | 0               | 5     | 4                        | 8.0 |

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| 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>       | %    |
| 1                             | 2               | 0               | 2               | 0               | 5     | 5                        | 10.0 |
| 0                             | 0               | 2               | 3               | 0               | 5     | 6                        | 12.0 |
| 1                             | 0               | 1               | 4               | 0               | 6     | 7                        | 14.0 |
| 0                             | 0               | 1               | 1               | 0               | 2     | 8                        | 16.0 |
| 0                             | 1               | 1               | 1               | 0               | 3     | 9                        | 18.0 |
| 0                             | 1               | 0               | 1               | 0               | 2     | 10                       | 20.0 |
| 0                             | 1               | 1               | 3               | 0               | 5     | 11                       | 22.0 |
| 0                             | 1               | 1               | 0               | 0               | 2     | 12                       | 24.0 |
| 0                             | 0               | 1               | 0               | 0               | 1     | 13                       | 26.0 |
| 0                             | 0               | 1               | 0               | 0               | 1     | 14                       | 28.0 |
| 0                             | 0               | 1               | 0               | 0               | 1     | 15                       | 30.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 16                       | 32.0 |
| 1                             | 0               | 1               | 0               | 0               | 2     | 17                       | 34.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 36.0 |
| 0                             | 0               | 0               | 1               | 0               | 1     | 19                       | 38.0 |
| 0                             | 1               | 0               | 0               | 0               | 1     | 20                       | 40.0 |
| 0                             | 0               | 1               | 0               | 0               | 1     | 21                       | 42.0 |
| 0                             | 0               | 1               | 0               | 0               | 1     | 22                       | 44.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 23                       | 46.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 24                       | 48.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 25                       | 50.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 26                       | 52.0 |
| 0                             | 0               | 0               | 1               | 0               | 1     | 27                       | 54.0 |
| 0                             | 1               | 0               | 1               | 0               | 2     | 28                       | 56.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 29                       | 58.0 |
| 0                             | 1               | 0               | 1               | 0               | 2     | 30                       | 60.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 31                       | 62.0 |
| 0                             | 0               | 0               | 1               | 0               | 1     | 32                       | 64.0 |
| 0                             | 2               | 0               | 0               | 0               | 2     | 33                       | 66.0 |
| 0                             | 1               | 0               | 0               | 0               | 1     | 34                       | 68.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 35                       | 70.0 |
| 0                             | 0               | 0               | 1               | 0               | 1     | 36                       | 72.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 37                       | 74.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 38                       | 76.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 39                       | 78.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 40                       | 80.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 41                       | 82.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 42                       | 84.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 43                       | 86.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 44                       | 88.0 |
| 0                             | 0               | 0               | 0               | 0               | 0     | 45                       | 90.0 |

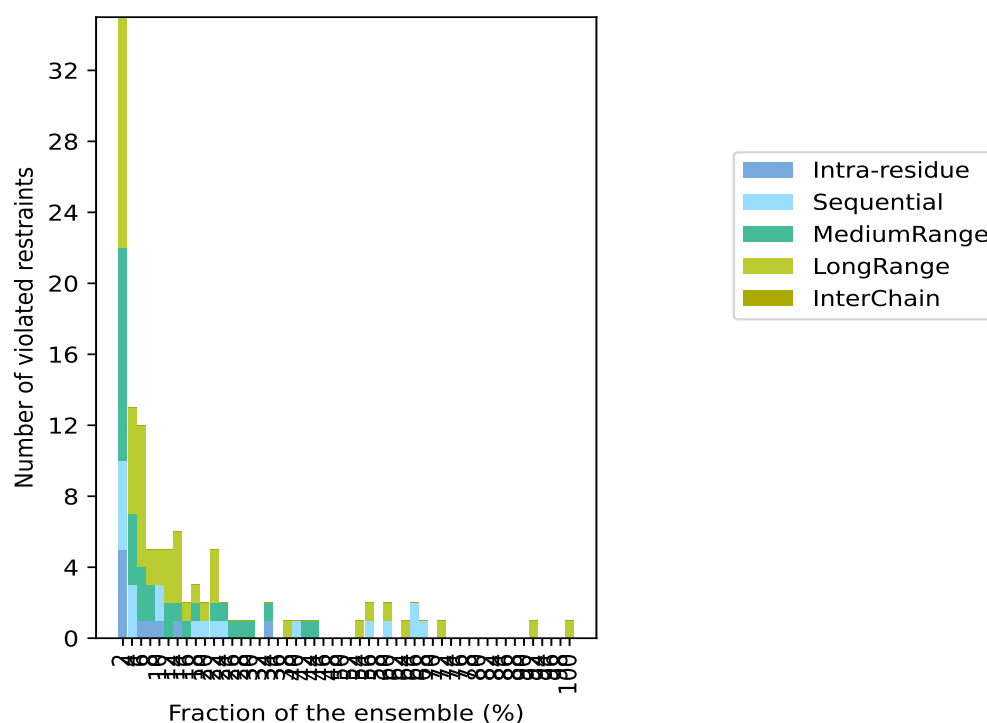
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 0                             | 0               | 0               | 1               | 0               | 1     | 46                       | 92.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 47                       | 94.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 48                       | 96.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 49                       | 98.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 50                       | 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

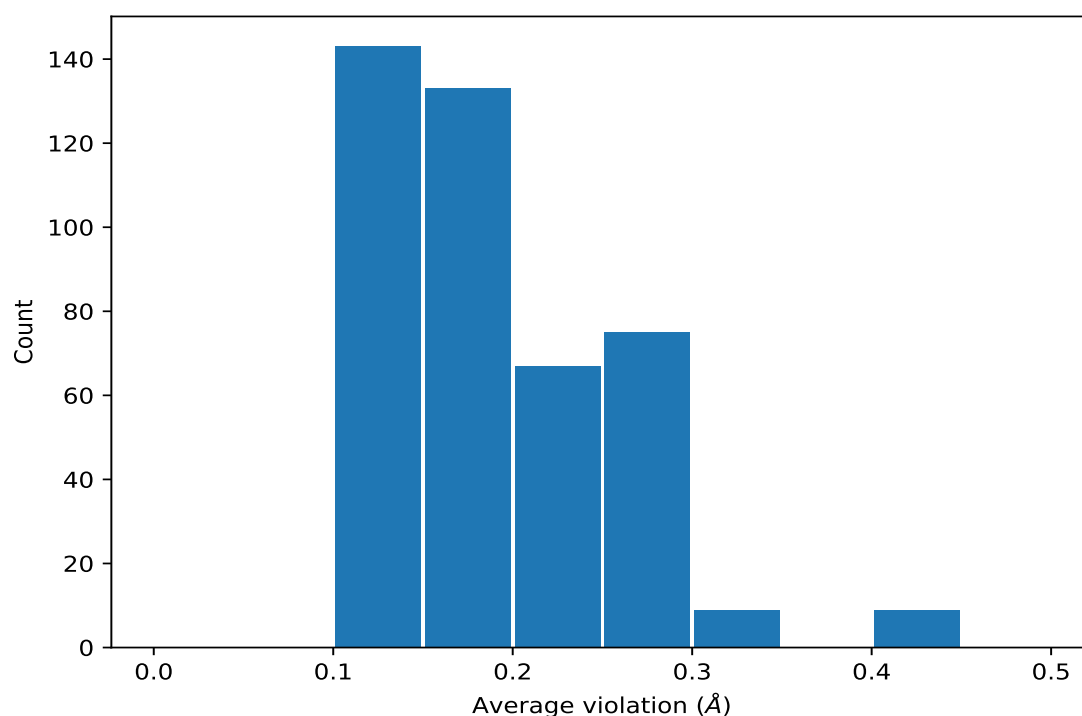
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 50                  | 0.27     | 0.09                | 0.26       |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 50                  | 0.27     | 0.09                | 0.26       |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 50                  | 0.27     | 0.09                | 0.26       |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 46                  | 0.32     | 0.11                | 0.3        |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 46                  | 0.32     | 0.11                | 0.3        |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 46                  | 0.32     | 0.11                | 0.3        |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 36                  | 0.28     | 0.08                | 0.27       |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 36                  | 0.28     | 0.08                | 0.27       |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 36                  | 0.28     | 0.08                | 0.27       |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 34                  | 0.27     | 0.07                | 0.26       |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 34                  | 0.27     | 0.07                | 0.26       |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 34                  | 0.27     | 0.07                | 0.26       |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 34                  | 0.27     | 0.07                | 0.26       |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 34                  | 0.27     | 0.07                | 0.26       |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 34                  | 0.27     | 0.07                | 0.26       |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 34                  | 0.27     | 0.07                | 0.26       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 34                  | 0.27     | 0.07                | 0.26       |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 34                  | 0.27     | 0.07                | 0.26       |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 33                  | 0.19     | 0.06                | 0.17       |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 33                  | 0.19     | 0.06                | 0.17       |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 33                  | 0.19     | 0.06                | 0.17       |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 33                  | 0.17     | 0.05                | 0.16       |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 32                  | 0.21     | 0.07                | 0.2        |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 32                  | 0.21     | 0.07                | 0.2        |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 32                  | 0.21     | 0.07                | 0.2        |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 30                  | 0.19     | 0.06                | 0.18       |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 30                  | 0.19     | 0.06                | 0.18       |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 30                  | 0.19     | 0.06                | 0.18       |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 30                  | 0.19     | 0.06                | 0.18       |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 30                  | 0.19     | 0.06                | 0.18       |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 30                  | 0.19     | 0.06                | 0.18       |
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 30                  | 0.17     | 0.05                | 0.16       |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 28                  | 0.2      | 0.06                | 0.19       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 28                  | 0.2      | 0.06                | 0.19       |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 28                  | 0.19     | 0.08                | 0.17       |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 28                  | 0.19     | 0.08                | 0.17       |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 28                  | 0.19     | 0.08                | 0.17       |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 28                  | 0.19     | 0.08                | 0.17       |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 28                  | 0.19     | 0.08                | 0.17       |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 28                  | 0.19     | 0.08                | 0.17       |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 27                  | 0.23     | 0.08                | 0.22       |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 22                  | 0.21     | 0.08                | 0.2        |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 22                  | 0.21     | 0.08                | 0.2        |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 22                  | 0.21     | 0.08                | 0.2        |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 21                  | 0.18     | 0.07                | 0.15       |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 21                  | 0.18     | 0.07                | 0.15       |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 21                  | 0.18     | 0.07                | 0.15       |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 20                  | 0.12     | 0.02                | 0.11       |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 20                  | 0.12     | 0.02                | 0.11       |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 20                  | 0.12     | 0.02                | 0.11       |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 20                  | 0.12     | 0.02                | 0.11       |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 19                  | 0.2      | 0.09                | 0.17       |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 19                  | 0.2      | 0.09                | 0.17       |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 19                  | 0.2      | 0.09                | 0.17       |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 19                  | 0.2      | 0.09                | 0.17       |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 19                  | 0.2      | 0.09                | 0.17       |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 19                  | 0.2      | 0.09                | 0.17       |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 19                  | 0.2      | 0.09                | 0.17       |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 19                  | 0.2      | 0.09                | 0.17       |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 19                  | 0.2      | 0.09                | 0.17       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 17                  | 0.16     | 0.05                | 0.16       |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 17                  | 0.15     | 0.03                | 0.14       |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 17                  | 0.15     | 0.03                | 0.14       |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 17                  | 0.15     | 0.03                | 0.14       |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 15                  | 0.18     | 0.07                | 0.16       |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 15                  | 0.18     | 0.07                | 0.16       |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 15                  | 0.18     | 0.07                | 0.16       |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 15                  | 0.18     | 0.07                | 0.16       |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 15                  | 0.18     | 0.07                | 0.16       |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 15                  | 0.18     | 0.07                | 0.16       |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 14                  | 0.14     | 0.03                | 0.12       |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 13                  | 0.17     | 0.05                | 0.15       |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 13                  | 0.17     | 0.05                | 0.15       |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 13                  | 0.17     | 0.05                | 0.15       |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 13                  | 0.17     | 0.05                | 0.15       |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 13                  | 0.17     | 0.05                | 0.15       |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 13                  | 0.17     | 0.05                | 0.15       |
| (1,435)  | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,435)  | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,435)  | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,435)  | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,435)  | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,435)  | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,435)  | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,435)  | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,435)  | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 12                  | 0.16     | 0.04                | 0.16       |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 12                  | 0.12     | 0.01                | 0.12       |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 12                  | 0.12     | 0.01                | 0.12       |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 12                  | 0.12     | 0.01                | 0.12       |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 12                  | 0.12     | 0.01                | 0.12       |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 12                  | 0.12     | 0.01                | 0.12       |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 12                  | 0.12     | 0.01                | 0.12       |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 11                  | 0.3      | 0.09                | 0.29       |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 11                  | 0.2      | 0.07                | 0.2        |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 11                  | 0.15     | 0.03                | 0.14       |
| (1,528)  | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 11                  | 0.14     | 0.02                | 0.14       |
| (1,528)  | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 11                  | 0.14     | 0.02                | 0.14       |
| (1,528)  | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 11                  | 0.14     | 0.02                | 0.14       |
| (1,542)  | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 11                  | 0.12     | 0.01                | 0.12       |
| (1,542)  | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 11                  | 0.12     | 0.01                | 0.12       |
| (1,542)  | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 11                  | 0.12     | 0.01                | 0.12       |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 10                  | 0.19     | 0.05                | 0.17       |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 10                  | 0.19     | 0.05                | 0.17       |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 10                  | 0.19     | 0.05                | 0.17       |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 10                  | 0.19     | 0.05                | 0.17       |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 10                  | 0.19     | 0.05                | 0.17       |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 10                  | 0.19     | 0.05                | 0.17       |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 10                  | 0.15     | 0.05                | 0.14       |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 10                  | 0.15     | 0.05                | 0.14       |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 10                  | 0.15     | 0.05                | 0.14       |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 10                  | 0.15     | 0.05                | 0.14       |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 10                  | 0.15     | 0.05                | 0.14       |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 10                  | 0.15     | 0.05                | 0.14       |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 9                   | 0.17     | 0.05                | 0.18       |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 9                   | 0.17     | 0.05                | 0.18       |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD11 | 9                   | 0.15     | 0.04                | 0.14       |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD12 | 9                   | 0.15     | 0.04                | 0.14       |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD13 | 9                   | 0.15     | 0.04                | 0.14       |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD21 | 9                   | 0.15     | 0.04                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD22 | 9                   | 0.15     | 0.04                | 0.14       |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD23 | 9                   | 0.15     | 0.04                | 0.14       |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 9                   | 0.14     | 0.03                | 0.13       |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 9                   | 0.14     | 0.03                | 0.13       |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 9                   | 0.14     | 0.03                | 0.13       |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 9                   | 0.14     | 0.03                | 0.13       |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 9                   | 0.14     | 0.03                | 0.13       |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 9                   | 0.14     | 0.03                | 0.13       |
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 8                   | 0.31     | 0.06                | 0.3        |
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 8                   | 0.31     | 0.06                | 0.3        |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 8                   | 0.31     | 0.06                | 0.3        |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 8                   | 0.31     | 0.06                | 0.3        |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 8                   | 0.31     | 0.06                | 0.3        |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 8                   | 0.31     | 0.06                | 0.3        |
| (1,451)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 8                   | 0.14     | 0.03                | 0.14       |
| (1,451)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 8                   | 0.14     | 0.03                | 0.14       |
| (1,451)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 8                   | 0.14     | 0.03                | 0.14       |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD11 | 7                   | 0.18     | 0.04                | 0.18       |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD12 | 7                   | 0.18     | 0.04                | 0.18       |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD13 | 7                   | 0.18     | 0.04                | 0.18       |
| (1,1067) | 1:49:A:LEU:HD11 | 1:54:A:LEU:H    | 7                   | 0.18     | 0.06                | 0.14       |
| (1,1067) | 1:49:A:LEU:HD12 | 1:54:A:LEU:H    | 7                   | 0.18     | 0.06                | 0.14       |
| (1,1067) | 1:49:A:LEU:HD13 | 1:54:A:LEU:H    | 7                   | 0.18     | 0.06                | 0.14       |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB2  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB3  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB2  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB3  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB2  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB3  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB2  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB3  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB2  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB3  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB2  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB3  | 7                   | 0.16     | 0.02                | 0.16       |
| (1,154)  | 1:20:A:ILE:HG21 | 1:29:A:MET:HA   | 7                   | 0.15     | 0.03                | 0.14       |
| (1,154)  | 1:20:A:ILE:HG22 | 1:29:A:MET:HA   | 7                   | 0.15     | 0.03                | 0.14       |
| (1,154)  | 1:20:A:ILE:HG23 | 1:29:A:MET:HA   | 7                   | 0.15     | 0.03                | 0.14       |
| (1,463)  | 1:49:A:LEU:HD11 | 1:55:A:GLY:H    | 7                   | 0.15     | 0.05                | 0.13       |
| (1,463)  | 1:49:A:LEU:HD12 | 1:55:A:GLY:H    | 7                   | 0.15     | 0.05                | 0.13       |
| (1,463)  | 1:49:A:LEU:HD13 | 1:55:A:GLY:H    | 7                   | 0.15     | 0.05                | 0.13       |
| (1,404)  | 1:44:A:ILE:H    | 1:44:A:ILE:HD11 | 7                   | 0.13     | 0.02                | 0.12       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,404)  | 1:44:A:ILE:H    | 1:44:A:ILE:HD12 | 7                   | 0.13     | 0.02                | 0.12       |
| (1,404)  | 1:44:A:ILE:H    | 1:44:A:ILE:HD13 | 7                   | 0.13     | 0.02                | 0.12       |
| (1,510)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD11 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,510)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD12 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,510)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD13 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,510)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD11 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,510)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD12 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,510)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD13 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,510)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD11 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,510)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD12 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,510)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD13 | 6                   | 0.43     | 0.08                | 0.48       |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD11 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD12 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD13 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD21 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD22 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD23 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD11 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD12 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD13 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD21 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD22 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD23 | 6                   | 0.19     | 0.05                | 0.2        |
| (1,456)  | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD11 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,456)  | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD12 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,456)  | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD13 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,456)  | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD11 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,456)  | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD12 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,456)  | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD13 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,456)  | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD11 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,456)  | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD12 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,456)  | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD13 | 6                   | 0.17     | 0.05                | 0.15       |
| (1,630)  | 1:63:A:LYS:HA   | 1:65:A:THR:HG21 | 6                   | 0.17     | 0.04                | 0.17       |
| (1,630)  | 1:63:A:LYS:HA   | 1:65:A:THR:HG22 | 6                   | 0.17     | 0.04                | 0.17       |
| (1,630)  | 1:63:A:LYS:HA   | 1:65:A:THR:HG23 | 6                   | 0.17     | 0.04                | 0.17       |
| (1,359)  | 1:39:A:LEU:HA   | 1:42:A:TYR:HB3  | 6                   | 0.15     | 0.02                | 0.16       |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD11 | 5                   | 0.27     | 0.16                | 0.17       |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD12 | 5                   | 0.27     | 0.16                | 0.17       |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD13 | 5                   | 0.27     | 0.16                | 0.17       |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD11 | 5                   | 0.27     | 0.16                | 0.17       |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD12 | 5                   | 0.27     | 0.16                | 0.17       |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD13 | 5                   | 0.27     | 0.16                | 0.17       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD11 | 5                   | 0.27     | 0.16                | 0.17       |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD12 | 5                   | 0.27     | 0.16                | 0.17       |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD13 | 5                   | 0.27     | 0.16                | 0.17       |
| (1,773)  | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE1  | 5                   | 0.24     | 0.1                 | 0.29       |
| (1,773)  | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE2  | 5                   | 0.24     | 0.1                 | 0.29       |
| (1,773)  | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE1  | 5                   | 0.24     | 0.1                 | 0.29       |
| (1,773)  | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE2  | 5                   | 0.24     | 0.1                 | 0.29       |
| (1,773)  | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE1  | 5                   | 0.24     | 0.1                 | 0.29       |
| (1,773)  | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE2  | 5                   | 0.24     | 0.1                 | 0.29       |
| (1,495)  | 1:53:A:ARG:HA   | 1:53:A:ARG:HD2  | 5                   | 0.16     | 0.05                | 0.15       |
| (1,495)  | 1:53:A:ARG:HA   | 1:53:A:ARG:HD3  | 5                   | 0.16     | 0.05                | 0.15       |
| (1,1737) | 1:68:A:GLU:HG2  | 1:69:A:GLU:H    | 5                   | 0.14     | 0.03                | 0.13       |
| (1,1737) | 1:68:A:GLU:HG3  | 1:69:A:GLU:H    | 5                   | 0.14     | 0.03                | 0.13       |
| (1,567)  | 1:58:A:ILE:HD11 | 1:59:A:ASN:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,567)  | 1:58:A:ILE:HD12 | 1:59:A:ASN:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,567)  | 1:58:A:ILE:HD13 | 1:59:A:ASN:H    | 5                   | 0.12     | 0.01                | 0.12       |
| (1,40)   | 1:12:A:ILE:HD11 | 1:39:A:LEU:HG   | 4                   | 0.16     | 0.07                | 0.12       |
| (1,40)   | 1:12:A:ILE:HD12 | 1:39:A:LEU:HG   | 4                   | 0.16     | 0.07                | 0.12       |
| (1,40)   | 1:12:A:ILE:HD13 | 1:39:A:LEU:HG   | 4                   | 0.16     | 0.07                | 0.12       |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD11 | 4                   | 0.15     | 0.02                | 0.15       |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD12 | 4                   | 0.15     | 0.02                | 0.15       |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD13 | 4                   | 0.15     | 0.02                | 0.15       |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD11 | 4                   | 0.15     | 0.02                | 0.15       |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD12 | 4                   | 0.15     | 0.02                | 0.15       |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD13 | 4                   | 0.15     | 0.02                | 0.15       |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE2  | 4                   | 0.14     | 0.03                | 0.15       |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE3  | 4                   | 0.14     | 0.03                | 0.15       |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD11 | 4                   | 0.12     | 0.02                | 0.11       |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD12 | 4                   | 0.12     | 0.02                | 0.11       |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD13 | 4                   | 0.12     | 0.02                | 0.11       |
| (1,360)  | 1:38:A:SER:H    | 1:42:A:TYR:HD1  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,360)  | 1:38:A:SER:H    | 1:42:A:TYR:HD2  | 4                   | 0.11     | 0.01                | 0.11       |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD11 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD12 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD13 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD21 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD22 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD23 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD11 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD12 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD13 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD21 | 3                   | 0.28     | 0.02                | 0.29       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD22 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD23 | 3                   | 0.28     | 0.02                | 0.29       |
| (1,625)  | 1:65:A:THR:HG21 | 1:70:A:LEU:HD11 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,625)  | 1:65:A:THR:HG21 | 1:70:A:LEU:HD12 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,625)  | 1:65:A:THR:HG21 | 1:70:A:LEU:HD13 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,625)  | 1:65:A:THR:HG22 | 1:70:A:LEU:HD11 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,625)  | 1:65:A:THR:HG22 | 1:70:A:LEU:HD12 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,625)  | 1:65:A:THR:HG22 | 1:70:A:LEU:HD13 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,625)  | 1:65:A:THR:HG23 | 1:70:A:LEU:HD11 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,625)  | 1:65:A:THR:HG23 | 1:70:A:LEU:HD12 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,625)  | 1:65:A:THR:HG23 | 1:70:A:LEU:HD13 | 3                   | 0.28     | 0.1                 | 0.22       |
| (1,1527) | 1:39:A:LEU:HD11 | 1:44:A:ILE:H    | 3                   | 0.26     | 0.08                | 0.27       |
| (1,1527) | 1:39:A:LEU:HD12 | 1:44:A:ILE:H    | 3                   | 0.26     | 0.08                | 0.27       |
| (1,1527) | 1:39:A:LEU:HD13 | 1:44:A:ILE:H    | 3                   | 0.26     | 0.08                | 0.27       |
| (1,1527) | 1:39:A:LEU:HD21 | 1:44:A:ILE:H    | 3                   | 0.26     | 0.08                | 0.27       |
| (1,1527) | 1:39:A:LEU:HD22 | 1:44:A:ILE:H    | 3                   | 0.26     | 0.08                | 0.27       |
| (1,1527) | 1:39:A:LEU:HD23 | 1:44:A:ILE:H    | 3                   | 0.26     | 0.08                | 0.27       |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD11 | 3                   | 0.25     | 0.1                 | 0.3        |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD12 | 3                   | 0.25     | 0.1                 | 0.3        |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD13 | 3                   | 0.25     | 0.1                 | 0.3        |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG11 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG12 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG13 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG21 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG22 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG23 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG11 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG12 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG13 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG21 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG22 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG23 | 3                   | 0.25     | 0.04                | 0.26       |
| (1,192)  | 1:26:A:ILE:HD11 | 1:32:A:VAL:H    | 3                   | 0.17     | 0.06                | 0.16       |
| (1,192)  | 1:26:A:ILE:HD12 | 1:32:A:VAL:H    | 3                   | 0.17     | 0.06                | 0.16       |
| (1,192)  | 1:26:A:ILE:HD13 | 1:32:A:VAL:H    | 3                   | 0.17     | 0.06                | 0.16       |
| (1,477)  | 1:49:A:LEU:H    | 1:49:A:LEU:HD21 | 3                   | 0.16     | 0.03                | 0.18       |
| (1,477)  | 1:49:A:LEU:H    | 1:49:A:LEU:HD22 | 3                   | 0.16     | 0.03                | 0.18       |
| (1,477)  | 1:49:A:LEU:H    | 1:49:A:LEU:HD23 | 3                   | 0.16     | 0.03                | 0.18       |
| (1,617)  | 1:60:A:ASP:HA   | 1:63:A:LYS:HB2  | 3                   | 0.16     | 0.03                | 0.15       |
| (1,617)  | 1:60:A:ASP:HA   | 1:63:A:LYS:HB3  | 3                   | 0.16     | 0.03                | 0.15       |
| (1,259)  | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,259)  | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 3                   | 0.14     | 0.01                | 0.14       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,259)  | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,259)  | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,259)  | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,259)  | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,259)  | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,259)  | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,259)  | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 3                   | 0.14     | 0.01                | 0.14       |
| (1,335)  | 1:36:A:ILE:HG21 | 1:77:A:LEU:H    | 3                   | 0.14     | 0.02                | 0.16       |
| (1,335)  | 1:36:A:ILE:HG22 | 1:77:A:LEU:H    | 3                   | 0.14     | 0.02                | 0.16       |
| (1,335)  | 1:36:A:ILE:HG23 | 1:77:A:LEU:H    | 3                   | 0.14     | 0.02                | 0.16       |
| (1,1576) | 1:46:A:LYS:HB2  | 1:85:A:ILE:HG21 | 3                   | 0.13     | 0.01                | 0.14       |
| (1,1576) | 1:46:A:LYS:HB2  | 1:85:A:ILE:HG22 | 3                   | 0.13     | 0.01                | 0.14       |
| (1,1576) | 1:46:A:LYS:HB2  | 1:85:A:ILE:HG23 | 3                   | 0.13     | 0.01                | 0.14       |
| (1,1576) | 1:46:A:LYS:HB3  | 1:85:A:ILE:HG21 | 3                   | 0.13     | 0.01                | 0.14       |
| (1,1576) | 1:46:A:LYS:HB3  | 1:85:A:ILE:HG22 | 3                   | 0.13     | 0.01                | 0.14       |
| (1,1576) | 1:46:A:LYS:HB3  | 1:85:A:ILE:HG23 | 3                   | 0.13     | 0.01                | 0.14       |
| (1,454)  | 1:49:A:LEU:HG   | 1:55:A:GLY:HA3  | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,370)  | 1:7:A:ALA:HB1   | 1:42:A:TYR:HE1  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,370)  | 1:7:A:ALA:HB1   | 1:42:A:TYR:HE2  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,370)  | 1:7:A:ALA:HB2   | 1:42:A:TYR:HE1  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,370)  | 1:7:A:ALA:HB2   | 1:42:A:TYR:HE2  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,370)  | 1:7:A:ALA:HB3   | 1:42:A:TYR:HE1  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,370)  | 1:7:A:ALA:HB3   | 1:42:A:TYR:HE2  | 2                   | 0.22     | 0.08                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HB2  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HB3  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HB2  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HB3  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HB2  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HB3  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HB2  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HB3  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HB2  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HB3  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HB2  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,1605) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HB3  | 2                   | 0.22     | 0.04                | 0.22       |
| (1,474)  | 1:49:A:LEU:HD21 | 1:81:A:TRP:HD1  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,474)  | 1:49:A:LEU:HD22 | 1:81:A:TRP:HD1  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,474)  | 1:49:A:LEU:HD23 | 1:81:A:TRP:HD1  | 2                   | 0.18     | 0.04                | 0.18       |
| (1,764)  | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG21 | 2                   | 0.18     | 0.08                | 0.18       |
| (1,764)  | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG22 | 2                   | 0.18     | 0.08                | 0.18       |
| (1,764)  | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG23 | 2                   | 0.18     | 0.08                | 0.18       |
| (1,764)  | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG21 | 2                   | 0.18     | 0.08                | 0.18       |

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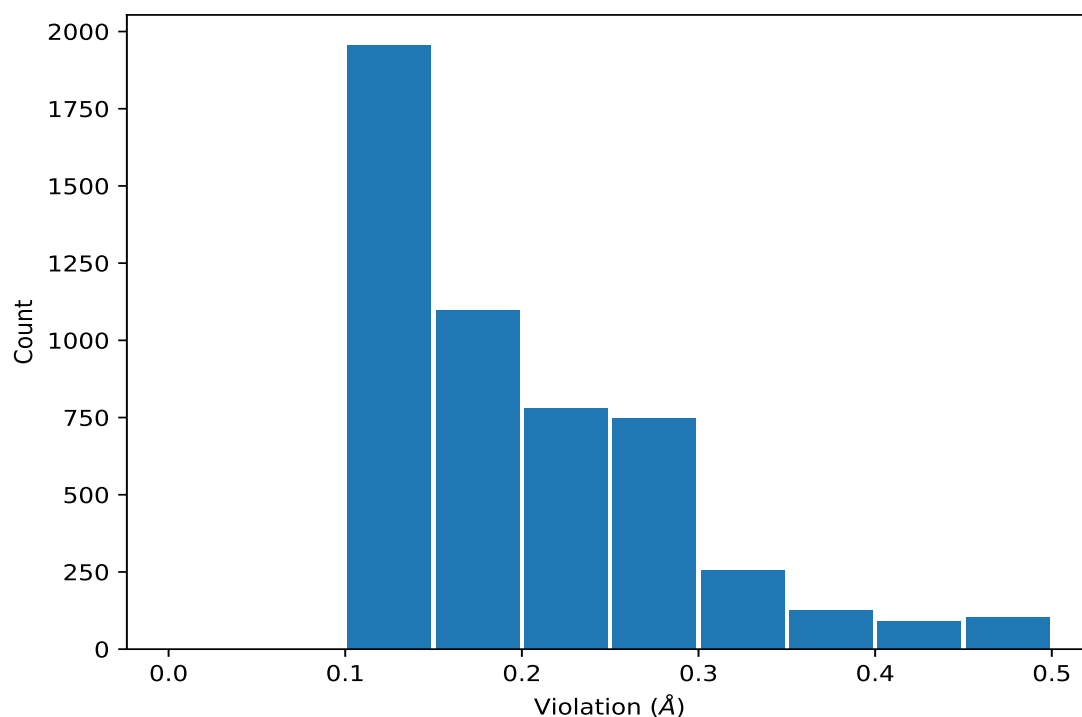
| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,764)  | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG22 | 2                   | 0.18     | 0.08                | 0.18       |
| (1,764)  | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG23 | 2                   | 0.18     | 0.08                | 0.18       |
| (1,427)  | 1:45:A:THR:HG21 | 1:46:A:LYS:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,427)  | 1:45:A:THR:HG22 | 1:46:A:LYS:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,427)  | 1:45:A:THR:HG23 | 1:46:A:LYS:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG11 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG12 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG13 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG21 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG22 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG23 | 2                   | 0.15     | 0.04                | 0.15       |
| (1,455)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD21 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,455)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD22 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,455)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD23 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,455)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD21 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,455)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD22 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,455)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD23 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,455)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD21 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,455)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD22 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,455)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD23 | 2                   | 0.14     | 0.03                | 0.14       |
| (1,701)  | 1:74:A:ALA:HA   | 1:77:A:LEU:HB3  | 2                   | 0.14     | 0.04                | 0.14       |
| (1,491)  | 1:51:A:GLU:H    | 1:52:A:THR:HG21 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,491)  | 1:51:A:GLU:H    | 1:52:A:THR:HG22 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,491)  | 1:51:A:GLU:H    | 1:52:A:THR:HG23 | 2                   | 0.14     | 0.01                | 0.14       |
| (1,655)  | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD21 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,655)  | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD22 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,655)  | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD23 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD11 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD12 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD13 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD21 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD22 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD23 | 2                   | 0.14     | 0.02                | 0.14       |
| (1,227)  | 1:26:A:ILE:HA   | 1:29:A:MET:HE1  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,227)  | 1:26:A:ILE:HA   | 1:29:A:MET:HE2  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,227)  | 1:26:A:ILE:HA   | 1:29:A:MET:HE3  | 2                   | 0.11     | 0.01                | 0.11       |
| (1,1562) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1562) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1562) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1562) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1562) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1562) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HB3  | 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) |
|---------|-----------------|-----------------|----------|---------------|
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD11 | 3        | 0.5           |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD12 | 3        | 0.5           |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD13 | 3        | 0.5           |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD11 | 3        | 0.5           |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD12 | 3        | 0.5           |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD13 | 3        | 0.5           |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD11 | 3        | 0.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD12 | 3        | 0.5           |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD13 | 3        | 0.5           |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD11 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD12 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD13 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD11 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD12 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD13 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD11 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD12 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD13 | 13       | 0.5           |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD11 | 22       | 0.49          |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD12 | 22       | 0.49          |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD13 | 22       | 0.49          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD11 | 22       | 0.49          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD12 | 22       | 0.49          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD13 | 22       | 0.49          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD11 | 22       | 0.49          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD12 | 22       | 0.49          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD13 | 22       | 0.49          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 31       | 0.49          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 31       | 0.49          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 31       | 0.49          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 32       | 0.48          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 32       | 0.48          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 32       | 0.48          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 43       | 0.48          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 43       | 0.48          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 43       | 0.48          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 39       | 0.48          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 39       | 0.48          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 39       | 0.48          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD11 | 15       | 0.47          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD12 | 15       | 0.47          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD13 | 15       | 0.47          |
| (1,749) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD11 | 15       | 0.47          |
| (1,749) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD12 | 15       | 0.47          |
| (1,749) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD13 | 15       | 0.47          |
| (1,749) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD11 | 15       | 0.47          |
| (1,749) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD12 | 15       | 0.47          |
| (1,749) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD13 | 15       | 0.47          |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD11 | 9        | 0.47          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD12 | 9        | 0.47          |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD13 | 9        | 0.47          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD11 | 9        | 0.47          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD12 | 9        | 0.47          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD13 | 9        | 0.47          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD11 | 9        | 0.47          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD12 | 9        | 0.47          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD13 | 9        | 0.47          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 39       | 0.46          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 39       | 0.46          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 39       | 0.46          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 19       | 0.46          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 19       | 0.46          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 19       | 0.46          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 46       | 0.46          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 46       | 0.46          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 46       | 0.46          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 50       | 0.46          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 50       | 0.46          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 50       | 0.46          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 48       | 0.46          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 48       | 0.46          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 48       | 0.46          |
| (1,407) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 48       | 0.46          |
| (1,407) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 48       | 0.46          |
| (1,407) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 48       | 0.46          |
| (1,407) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 48       | 0.46          |
| (1,407) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 48       | 0.46          |
| (1,407) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 48       | 0.46          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 18       | 0.46          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 18       | 0.46          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 18       | 0.46          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 18       | 0.46          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 18       | 0.46          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 18       | 0.46          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 18       | 0.46          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 18       | 0.46          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 18       | 0.46          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD11 | 46       | 0.45          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD12 | 46       | 0.45          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD13 | 46       | 0.45          |
| (1,749) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD11 | 46       | 0.45          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD12 | 46       | 0.45          |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD13 | 46       | 0.45          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD11 | 46       | 0.45          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD12 | 46       | 0.45          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD13 | 46       | 0.45          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 24       | 0.45          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 24       | 0.45          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 24       | 0.45          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 47       | 0.45          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 47       | 0.45          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 47       | 0.45          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 17       | 0.44          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 17       | 0.44          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 17       | 0.44          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 37       | 0.44          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 37       | 0.44          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 37       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 35       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 35       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 35       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 35       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 35       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 35       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 35       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 35       | 0.44          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 35       | 0.44          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 38       | 0.43          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 38       | 0.43          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 38       | 0.43          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 41       | 0.43          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 41       | 0.43          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 41       | 0.43          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 44       | 0.43          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 44       | 0.43          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 44       | 0.43          |
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 46       | 0.42          |
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 46       | 0.42          |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 46       | 0.42          |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 46       | 0.42          |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 46       | 0.42          |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 46       | 0.42          |
| (1,625)  | 1:65:A:THR:HG21 | 1:70:A:LEU:HD11 | 44       | 0.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,625) | 1:65:A:THR:HG21 | 1:70:A:LEU:HD12 | 44       | 0.42          |
| (1,625) | 1:65:A:THR:HG21 | 1:70:A:LEU:HD13 | 44       | 0.42          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD11 | 44       | 0.42          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD12 | 44       | 0.42          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD13 | 44       | 0.42          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD11 | 44       | 0.42          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD12 | 44       | 0.42          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD13 | 44       | 0.42          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 37       | 0.42          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 37       | 0.42          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 37       | 0.42          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 25       | 0.42          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 25       | 0.42          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 25       | 0.42          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 29       | 0.42          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 29       | 0.42          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 29       | 0.42          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 42       | 0.42          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 42       | 0.42          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 42       | 0.42          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 48       | 0.42          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 48       | 0.42          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 48       | 0.42          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 48       | 0.42          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 48       | 0.42          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 48       | 0.42          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 48       | 0.42          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 48       | 0.42          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 48       | 0.42          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 43       | 0.41          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 43       | 0.41          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 43       | 0.41          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 34       | 0.41          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 34       | 0.41          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 34       | 0.41          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 34       | 0.41          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 34       | 0.41          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 34       | 0.41          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 34       | 0.41          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 34       | 0.41          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 34       | 0.41          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 36       | 0.41          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 36       | 0.41          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 36       | 0.41          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 48       | 0.41          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 48       | 0.41          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 48       | 0.41          |
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 44       | 0.4           |
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 44       | 0.4           |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 44       | 0.4           |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 44       | 0.4           |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 44       | 0.4           |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 44       | 0.4           |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 26       | 0.4           |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 26       | 0.4           |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 26       | 0.4           |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 45       | 0.4           |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 45       | 0.4           |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 45       | 0.4           |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 48       | 0.39          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 48       | 0.39          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 48       | 0.39          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 23       | 0.39          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 23       | 0.39          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 23       | 0.39          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 34       | 0.39          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 34       | 0.39          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 34       | 0.39          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 39       | 0.39          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 39       | 0.39          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 39       | 0.39          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 41       | 0.38          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 41       | 0.38          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 41       | 0.38          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 41       | 0.38          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 41       | 0.38          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 41       | 0.38          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 41       | 0.38          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 41       | 0.38          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 41       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 24       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 24       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 24       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 30       | 0.38          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 30       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 30       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 41       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 41       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 41       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 49       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 49       | 0.38          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 49       | 0.38          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 45       | 0.37          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 45       | 0.37          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 45       | 0.37          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 45       | 0.37          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 45       | 0.37          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 45       | 0.37          |
| (1,773)  | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE1  | 37       | 0.37          |
| (1,773)  | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE2  | 37       | 0.37          |
| (1,773)  | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE1  | 37       | 0.37          |
| (1,773)  | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE2  | 37       | 0.37          |
| (1,773)  | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE1  | 37       | 0.37          |
| (1,773)  | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE2  | 37       | 0.37          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 50       | 0.37          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 50       | 0.37          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 50       | 0.37          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 27       | 0.37          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 27       | 0.37          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 27       | 0.37          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 30       | 0.37          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 30       | 0.37          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 30       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 38       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 38       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 38       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 38       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 38       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 38       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 38       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 38       | 0.37          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 38       | 0.37          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 37       | 0.36          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 37       | 0.36          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 37       | 0.36          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 37       | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 37       | 0.36          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 37       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 28       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 28       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 28       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 30       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 30       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 30       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 48       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 48       | 0.36          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 48       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD11 | 11       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD12 | 11       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD13 | 11       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD11 | 11       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD12 | 11       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD13 | 11       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD11 | 11       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD12 | 11       | 0.36          |
| (1,510)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD13 | 11       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 15       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 49       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 50       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 50       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 50       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 50       | 0.36          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 50       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 50       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 50       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 50       | 0.36          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 50       | 0.36          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 36       | 0.36          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 36       | 0.36          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 36       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 50       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 50       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 50       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 50       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 50       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 50       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 50       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 50       | 0.36          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 50       | 0.36          |
| (1,1527) | 1:39:A:LEU:HD11 | 1:44:A:ILE:H    | 43       | 0.35          |
| (1,1527) | 1:39:A:LEU:HD12 | 1:44:A:ILE:H    | 43       | 0.35          |
| (1,1527) | 1:39:A:LEU:HD13 | 1:44:A:ILE:H    | 43       | 0.35          |
| (1,1527) | 1:39:A:LEU:HD21 | 1:44:A:ILE:H    | 43       | 0.35          |
| (1,1527) | 1:39:A:LEU:HD22 | 1:44:A:ILE:H    | 43       | 0.35          |
| (1,1527) | 1:39:A:LEU:HD23 | 1:44:A:ILE:H    | 43       | 0.35          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 46       | 0.35          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 46       | 0.35          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 46       | 0.35          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 46       | 0.35          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 46       | 0.35          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 46       | 0.35          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 40       | 0.35          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 40       | 0.35          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 40       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 27       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 27       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 27       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 27       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 27       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 27       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 27       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 27       | 0.35          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 27       | 0.35          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 23       | 0.35          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 23       | 0.35          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 23       | 0.35          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 21       | 0.35          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 21       | 0.35          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 21       | 0.35          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 25       | 0.35          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 25       | 0.35          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 25       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 44       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 44       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 44       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 44       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 44       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 44       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 44       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 44       | 0.35          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 44       | 0.35          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 46       | 0.35          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 46       | 0.35          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 46       | 0.35          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 46       | 0.35          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 46       | 0.35          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 46       | 0.35          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 46       | 0.35          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 46       | 0.35          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 46       | 0.35          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 26       | 0.34          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 26       | 0.34          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 26       | 0.34          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 26       | 0.34          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 26       | 0.34          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 26       | 0.34          |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD11 | 49       | 0.34          |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD12 | 49       | 0.34          |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD13 | 49       | 0.34          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 21       | 0.34          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 21       | 0.34          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 21       | 0.34          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 42       | 0.34          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 42       | 0.34          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 42       | 0.34          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 42       | 0.34          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 42       | 0.34          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 42       | 0.34          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 42       | 0.34          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 42       | 0.34          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 42       | 0.34          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 35       | 0.34          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 35       | 0.34          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 35       | 0.34          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 19       | 0.34          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 19       | 0.34          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 19       | 0.34          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 31       | 0.34          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 31       | 0.34          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 31       | 0.34          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 31       | 0.34          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 31       | 0.34          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 31       | 0.34          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 31       | 0.34          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 23       | 0.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 23       | 0.33          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 23       | 0.33          |
| (1,1434) | 1:29:A:MET:HG2  | 1:70:A:LEU:HD11 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG2  | 1:70:A:LEU:HD12 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG2  | 1:70:A:LEU:HD13 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG2  | 1:70:A:LEU:HD21 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG2  | 1:70:A:LEU:HD22 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG2  | 1:70:A:LEU:HD23 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG3  | 1:70:A:LEU:HD11 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG3  | 1:70:A:LEU:HD12 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG3  | 1:70:A:LEU:HD13 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG3  | 1:70:A:LEU:HD21 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG3  | 1:70:A:LEU:HD22 | 47       | 0.33          |
| (1,1434) | 1:29:A:MET:HG3  | 1:70:A:LEU:HD23 | 47       | 0.33          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 43       | 0.33          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 43       | 0.33          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 43       | 0.33          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 27       | 0.33          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 27       | 0.33          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 27       | 0.33          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 29       | 0.33          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 29       | 0.33          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 29       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 43       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 48       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 48       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 48       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 48       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 48       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 48       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 48       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 48       | 0.33          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 48       | 0.33          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 37       | 0.33          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 37       | 0.33          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 37       | 0.33          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 32       | 0.33          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 32       | 0.33          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 32       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 38       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 38       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 38       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 38       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 38       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 38       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 38       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 38       | 0.33          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 38       | 0.33          |
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 32       | 0.32          |
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 32       | 0.32          |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 32       | 0.32          |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 32       | 0.32          |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 32       | 0.32          |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 32       | 0.32          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 47       | 0.32          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 18       | 0.32          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 18       | 0.32          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 18       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 5        | 0.32          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 37       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 37       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 37       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 37       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 37       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 37       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 37       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 37       | 0.32          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 37       | 0.32          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 40       | 0.32          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 40       | 0.32          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 40       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 4        | 0.32          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 35       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 35       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 35       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 35       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 35       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 35       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 35       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 35       | 0.32          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 35       | 0.32          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 14       | 0.31          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 14       | 0.31          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 14       | 0.31          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 14       | 0.31          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 14       | 0.31          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 14       | 0.31          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 26       | 0.31          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 26       | 0.31          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 26       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 46       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 46       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 46       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 46       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 46       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 46       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 46       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 46       | 0.31          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 46       | 0.31          |
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 49       | 0.31          |
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 49       | 0.31          |
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 49       | 0.31          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 49       | 0.31          |
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 49       | 0.31          |
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 49       | 0.31          |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 49       | 0.31          |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 49       | 0.31          |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 49       | 0.31          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 27       | 0.31          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 27       | 0.31          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 27       | 0.31          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 45       | 0.31          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 45       | 0.31          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 45       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 20       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 20       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 20       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 20       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 20       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 20       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 20       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 20       | 0.31          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 20       | 0.31          |
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 3        | 0.3           |
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 3        | 0.3           |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 3        | 0.3           |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 3        | 0.3           |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 3        | 0.3           |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 3        | 0.3           |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD11 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD12 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD13 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD21 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD22 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD23 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD11 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD12 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD13 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD21 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD22 | 47       | 0.3           |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD23 | 47       | 0.3           |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 37       | 0.3           |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 37       | 0.3           |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 37       | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 37       | 0.3           |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 37       | 0.3           |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 37       | 0.3           |
| (1,773)  | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE1  | 44       | 0.3           |
| (1,773)  | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE2  | 44       | 0.3           |
| (1,773)  | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE1  | 44       | 0.3           |
| (1,773)  | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE2  | 44       | 0.3           |
| (1,773)  | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE1  | 44       | 0.3           |
| (1,773)  | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE2  | 44       | 0.3           |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD11 | 43       | 0.3           |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD12 | 43       | 0.3           |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD13 | 43       | 0.3           |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 31       | 0.3           |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 31       | 0.3           |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 31       | 0.3           |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 35       | 0.3           |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 35       | 0.3           |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 35       | 0.3           |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 28       | 0.3           |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 28       | 0.3           |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 28       | 0.3           |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 40       | 0.3           |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 40       | 0.3           |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 40       | 0.3           |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 4        | 0.3           |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 4        | 0.3           |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 4        | 0.3           |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 23       | 0.3           |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 23       | 0.3           |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 23       | 0.3           |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 30       | 0.3           |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 30       | 0.3           |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 30       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 18       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 18       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 18       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 18       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 18       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 18       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 18       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 18       | 0.3           |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 18       | 0.3           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,370)  | 1:7:A:ALA:HB1   | 1:42:A:TYR:HE1  | 40       | 0.3           |
| (1,370)  | 1:7:A:ALA:HB1   | 1:42:A:TYR:HE2  | 40       | 0.3           |
| (1,370)  | 1:7:A:ALA:HB2   | 1:42:A:TYR:HE1  | 40       | 0.3           |
| (1,370)  | 1:7:A:ALA:HB2   | 1:42:A:TYR:HE2  | 40       | 0.3           |
| (1,370)  | 1:7:A:ALA:HB3   | 1:42:A:TYR:HE1  | 40       | 0.3           |
| (1,370)  | 1:7:A:ALA:HB3   | 1:42:A:TYR:HE2  | 40       | 0.3           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 40       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 40       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 15       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 15       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 15       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 15       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 15       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 15       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 34       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 34       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 34       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 34       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 34       | 0.29          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 34       | 0.29          |
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 45       | 0.29          |
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 45       | 0.29          |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 45       | 0.29          |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 45       | 0.29          |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 45       | 0.29          |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 45       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD11 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD12 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD13 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD21 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD22 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD23 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD11 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD12 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD13 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD21 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD22 | 22       | 0.29          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD23 | 22       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG11 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG12 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG13 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG21 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG22 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG23 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG11 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG12 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG13 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG21 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG22 | 40       | 0.29          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG23 | 40       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 21       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 21       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 21       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 21       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 21       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 21       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 49       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 49       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 49       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 49       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 49       | 0.29          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 49       | 0.29          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 41       | 0.29          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 41       | 0.29          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 41       | 0.29          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 41       | 0.29          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 41       | 0.29          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 41       | 0.29          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,773) | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE1  | 43       | 0.29          |
| (1,773) | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE2  | 43       | 0.29          |
| (1,773) | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE1  | 43       | 0.29          |
| (1,773) | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE2  | 43       | 0.29          |
| (1,773) | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE1  | 43       | 0.29          |
| (1,773) | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE2  | 43       | 0.29          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 15       | 0.29          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 15       | 0.29          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 15       | 0.29          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 44       | 0.29          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 44       | 0.29          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 44       | 0.29          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 38       | 0.29          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 38       | 0.29          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 38       | 0.29          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 38       | 0.29          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 38       | 0.29          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 38       | 0.29          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 38       | 0.29          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 38       | 0.29          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 38       | 0.29          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 14       | 0.29          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 14       | 0.29          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 14       | 0.29          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 14       | 0.29          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 14       | 0.29          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 14       | 0.29          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 14       | 0.29          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 14       | 0.29          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 14       | 0.29          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 33       | 0.29          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 33       | 0.29          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 33       | 0.29          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 47       | 0.29          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 47       | 0.29          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 47       | 0.29          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 29       | 0.29          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 29       | 0.29          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 29       | 0.29          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 44       | 0.29          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 44       | 0.29          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 44       | 0.29          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 44       | 0.29          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 44       | 0.29          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 44       | 0.29          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 44       | 0.29          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 44       | 0.29          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 44       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 14       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 14       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 14       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 14       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 14       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 14       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 14       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 14       | 0.29          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 14       | 0.29          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 32       | 0.29          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 41       | 0.29          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 41       | 0.29          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 41       | 0.29          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 41       | 0.29          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 41       | 0.29          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 41       | 0.29          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 41       | 0.29          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 41       | 0.29          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 41       | 0.29          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 33       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 33       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 41       | 0.28          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 41       | 0.28          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 50       | 0.28          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 19       | 0.28          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 19       | 0.28          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 19       | 0.28          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 45       | 0.28          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 45       | 0.28          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 45       | 0.28          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 16       | 0.28          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 16       | 0.28          |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 16       | 0.28          |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 16       | 0.28          |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 16       | 0.28          |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 16       | 0.28          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 24       | 0.28          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 24       | 0.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 24       | 0.28          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 42       | 0.28          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 42       | 0.28          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 42       | 0.28          |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD11 | 10       | 0.28          |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD12 | 10       | 0.28          |
| (1,510) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD13 | 10       | 0.28          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD11 | 10       | 0.28          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD12 | 10       | 0.28          |
| (1,510) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD13 | 10       | 0.28          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD11 | 10       | 0.28          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD12 | 10       | 0.28          |
| (1,510) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD13 | 10       | 0.28          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 26       | 0.28          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 26       | 0.28          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 26       | 0.28          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 26       | 0.28          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 26       | 0.28          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 26       | 0.28          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 26       | 0.28          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 26       | 0.28          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 26       | 0.28          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 26       | 0.28          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 26       | 0.28          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 26       | 0.28          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 34       | 0.28          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 34       | 0.28          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 34       | 0.28          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 48       | 0.28          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 48       | 0.28          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 48       | 0.28          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 17       | 0.28          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 17       | 0.28          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 17       | 0.28          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 36       | 0.28          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 36       | 0.28          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 36       | 0.28          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 25       | 0.28          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 25       | 0.28          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 25       | 0.28          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 25       | 0.28          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 25       | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 25       | 0.28          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 25       | 0.28          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 25       | 0.28          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 25       | 0.28          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 29       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 29       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 29       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 29       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 29       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 29       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 32       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 32       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 32       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 32       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 32       | 0.27          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 32       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 17       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 46       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 46       | 0.27          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 46       | 0.27          |
| (1,1527) | 1:39:A:LEU:HD11 | 1:44:A:ILE:H    | 49       | 0.27          |
| (1,1527) | 1:39:A:LEU:HD12 | 1:44:A:ILE:H    | 49       | 0.27          |
| (1,1527) | 1:39:A:LEU:HD13 | 1:44:A:ILE:H    | 49       | 0.27          |
| (1,1527) | 1:39:A:LEU:HD21 | 1:44:A:ILE:H    | 49       | 0.27          |
| (1,1527) | 1:39:A:LEU:HD22 | 1:44:A:ILE:H    | 49       | 0.27          |
| (1,1527) | 1:39:A:LEU:HD23 | 1:44:A:ILE:H    | 49       | 0.27          |
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 42       | 0.27          |
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 42       | 0.27          |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 42       | 0.27          |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 42       | 0.27          |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 42       | 0.27          |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 42       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 45       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 45       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 45       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 45       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 45       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 45       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 46       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 46       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 46       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 46       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 46       | 0.27          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 46       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD11 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD12 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD13 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD21 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD22 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD23 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD11 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD12 | 48       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD13 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD21 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD22 | 48       | 0.27          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD23 | 48       | 0.27          |
| (1,1067) | 1:49:A:LEU:HD11 | 1:54:A:LEU:H    | 49       | 0.27          |
| (1,1067) | 1:49:A:LEU:HD12 | 1:54:A:LEU:H    | 49       | 0.27          |
| (1,1067) | 1:49:A:LEU:HD13 | 1:54:A:LEU:H    | 49       | 0.27          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 48       | 0.27          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 29       | 0.27          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 29       | 0.27          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 29       | 0.27          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 36       | 0.27          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 36       | 0.27          |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 36       | 0.27          |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 36       | 0.27          |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 36       | 0.27          |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 36       | 0.27          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 19       | 0.27          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 19       | 0.27          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 19       | 0.27          |
| (1,456)  | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD11 | 2        | 0.27          |
| (1,456)  | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD12 | 2        | 0.27          |
| (1,456)  | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD13 | 2        | 0.27          |
| (1,456)  | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD11 | 2        | 0.27          |
| (1,456)  | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD12 | 2        | 0.27          |
| (1,456)  | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD13 | 2        | 0.27          |
| (1,456)  | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD11 | 2        | 0.27          |
| (1,456)  | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD12 | 2        | 0.27          |
| (1,456)  | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD13 | 2        | 0.27          |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 45       | 0.27          |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 45       | 0.27          |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 45       | 0.27          |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 45       | 0.27          |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 45       | 0.27          |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 45       | 0.27          |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 45       | 0.27          |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 45       | 0.27          |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 45       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 19       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 19       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 19       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 19       | 0.27          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 19       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 19       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 19       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 19       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 19       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 29       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 29       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 29       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 29       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 29       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 29       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 29       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 29       | 0.27          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 29       | 0.27          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 15       | 0.27          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 15       | 0.27          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 15       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 15       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 15       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 15       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 37       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 37       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 37       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 41       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 41       | 0.27          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 41       | 0.27          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 38       | 0.27          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 38       | 0.27          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 38       | 0.27          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 49       | 0.27          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 49       | 0.27          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 49       | 0.27          |
| (1,40)   | 1:12:A:ILE:HD11 | 1:39:A:LEU:HG   | 45       | 0.27          |
| (1,40)   | 1:12:A:ILE:HD12 | 1:39:A:LEU:HG   | 45       | 0.27          |
| (1,40)   | 1:12:A:ILE:HD13 | 1:39:A:LEU:HG   | 45       | 0.27          |
| (1,1619) | 1:51:A:GLU:HG2  | 1:52:A:THR:HG21 | 14       | 0.26          |
| (1,1619) | 1:51:A:GLU:HG2  | 1:52:A:THR:HG22 | 14       | 0.26          |
| (1,1619) | 1:51:A:GLU:HG2  | 1:52:A:THR:HG23 | 14       | 0.26          |
| (1,1619) | 1:51:A:GLU:HG3  | 1:52:A:THR:HG21 | 14       | 0.26          |
| (1,1619) | 1:51:A:GLU:HG3  | 1:52:A:THR:HG22 | 14       | 0.26          |
| (1,1619) | 1:51:A:GLU:HG3  | 1:52:A:THR:HG23 | 14       | 0.26          |
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 8        | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 8        | 0.26          |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 8        | 0.26          |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 8        | 0.26          |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 8        | 0.26          |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD11 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD12 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD13 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD21 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD22 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG2  | 1:33:A:LEU:HD23 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD11 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD12 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD13 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD21 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD22 | 8        | 0.26          |
| (1,1433) | 1:29:A:MET:HG3  | 1:33:A:LEU:HD23 | 8        | 0.26          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG11 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG12 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG13 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG21 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG22 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG23 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG11 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG12 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG13 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG21 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG22 | 34       | 0.26          |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG23 | 34       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 27       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 27       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 27       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 27       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 27       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 27       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 28       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 28       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 28       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 28       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 28       | 0.26          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 28       | 0.26          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 49       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 49       | 0.26          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 49       | 0.26          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 49       | 0.26          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 49       | 0.26          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 49       | 0.26          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 40       | 0.26          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 40       | 0.26          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 40       | 0.26          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD11 | 38       | 0.26          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD12 | 38       | 0.26          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD13 | 38       | 0.26          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 4        | 0.26          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 4        | 0.26          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 4        | 0.26          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 38       | 0.26          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 38       | 0.26          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 38       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 18       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 18       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 18       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 18       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 18       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 18       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 18       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 18       | 0.26          |
| (1,424)  | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 18       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 18       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 18       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 18       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 21       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 21       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 21       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 48       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 48       | 0.26          |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 48       | 0.26          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 25       | 0.26          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 25       | 0.26          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 25       | 0.26          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 40       | 0.26          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 40       | 0.26          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 40       | 0.26          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 16       | 0.26          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 16       | 0.26          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 16       | 0.26          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 33       | 0.26          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 33       | 0.26          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 33       | 0.26          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 4        | 0.26          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 4        | 0.26          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 4        | 0.26          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 4        | 0.26          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 4        | 0.26          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 4        | 0.26          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 4        | 0.26          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 4        | 0.26          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 4        | 0.26          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 25       | 0.26          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 25       | 0.26          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 25       | 0.26          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 34       | 0.26          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 34       | 0.26          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 34       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 47       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 47       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 47       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 47       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 47       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 47       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 47       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 47       | 0.26          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 47       | 0.26          |
| (1,1605) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HB2  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HB3  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HB2  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HB3  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HB2  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HB3  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HB2  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HB3  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HB2  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HB3  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HB2  | 21       | 0.25          |
| (1,1605) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HB3  | 21       | 0.25          |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 41       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 41       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 19       | 0.25          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 19       | 0.25          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD11 | 26       | 0.25          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD12 | 26       | 0.25          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD13 | 26       | 0.25          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD21 | 26       | 0.25          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD22 | 26       | 0.25          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD23 | 26       | 0.25          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 43       | 0.25          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 43       | 0.25          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 43       | 0.25          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 43       | 0.25          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 43       | 0.25          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 43       | 0.25          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 39       | 0.25          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 39       | 0.25          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 39       | 0.25          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 15       | 0.25          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 15       | 0.25          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 15       | 0.25          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 21       | 0.25          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 21       | 0.25          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 21       | 0.25          |
| (1,764)  | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG21 | 20       | 0.25          |
| (1,764)  | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG22 | 20       | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,764) | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG23 | 20       | 0.25          |
| (1,764) | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG21 | 20       | 0.25          |
| (1,764) | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG22 | 20       | 0.25          |
| (1,764) | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG23 | 20       | 0.25          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 13       | 0.25          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 13       | 0.25          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 13       | 0.25          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 17       | 0.25          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 17       | 0.25          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 17       | 0.25          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 47       | 0.25          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 47       | 0.25          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 47       | 0.25          |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD2  | 1        | 0.25          |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD3  | 1        | 0.25          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 14       | 0.25          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 40       | 0.25          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 40       | 0.25          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 40       | 0.25          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 40       | 0.25          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 40       | 0.25          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 40       | 0.25          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 40       | 0.25          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 40       | 0.25          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 40       | 0.25          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 12       | 0.25          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 12       | 0.25          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 12       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 12       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 12       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 12       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 12       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 12       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 12       | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 25       | 0.25          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 32       | 0.25          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 32       | 0.25          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 32       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 32       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 32       | 0.25          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 32       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 32       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 32       | 0.25          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 32       | 0.25          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 18       | 0.25          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 18       | 0.25          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 18       | 0.25          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 18       | 0.25          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 18       | 0.25          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 18       | 0.25          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 18       | 0.25          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 18       | 0.25          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 18       | 0.25          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 2        | 0.25          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 2        | 0.25          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 2        | 0.25          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 18       | 0.25          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 18       | 0.25          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 18       | 0.25          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 21       | 0.25          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 21       | 0.25          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 21       | 0.25          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 40       | 0.25          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 40       | 0.25          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 40       | 0.25          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 41       | 0.25          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 41       | 0.25          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 41       | 0.25          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 19       | 0.25          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 19       | 0.25          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 19       | 0.25          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 19       | 0.25          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 19       | 0.25          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 19       | 0.25          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 19       | 0.25          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 19       | 0.25          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 19       | 0.25          |
| (1,192)  | 1:26:A:ILE:HD11 | 1:32:A:VAL:H    | 28       | 0.25          |
| (1,192)  | 1:26:A:ILE:HD12 | 1:32:A:VAL:H    | 28       | 0.25          |
| (1,192)  | 1:26:A:ILE:HD13 | 1:32:A:VAL:H    | 28       | 0.25          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 29       | 0.24          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 29       | 0.24          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 29       | 0.24          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 29       | 0.24          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 29       | 0.24          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 29       | 0.24          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 13       | 0.24          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 13       | 0.24          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 13       | 0.24          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 13       | 0.24          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 13       | 0.24          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 13       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG11 | 1:36:A:ILE:HD11 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG11 | 1:36:A:ILE:HD12 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG11 | 1:36:A:ILE:HD13 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG12 | 1:36:A:ILE:HD11 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG12 | 1:36:A:ILE:HD12 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG12 | 1:36:A:ILE:HD13 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG13 | 1:36:A:ILE:HD11 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG13 | 1:36:A:ILE:HD12 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG13 | 1:36:A:ILE:HD13 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG21 | 1:36:A:ILE:HD11 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG21 | 1:36:A:ILE:HD12 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG21 | 1:36:A:ILE:HD13 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG22 | 1:36:A:ILE:HD11 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG22 | 1:36:A:ILE:HD12 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG22 | 1:36:A:ILE:HD13 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG23 | 1:36:A:ILE:HD11 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG23 | 1:36:A:ILE:HD12 | 40       | 0.24          |
| (1,1484) | 1:35:A:VAL:HG23 | 1:36:A:ILE:HD13 | 40       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 32       | 0.24          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 32       | 0.24          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 32       | 0.24          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 32       | 0.24          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 32       | 0.24          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 32       | 0.24          |
| (1,1067) | 1:49:A:LEU:HD11 | 1:54:A:LEU:H    | 43       | 0.24          |
| (1,1067) | 1:49:A:LEU:HD12 | 1:54:A:LEU:H    | 43       | 0.24          |
| (1,1067) | 1:49:A:LEU:HD13 | 1:54:A:LEU:H    | 43       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD21 | 28       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD22 | 28       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD21 | 1:84:A:LEU:HD23 | 28       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD21 | 28       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD22 | 28       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD22 | 1:84:A:LEU:HD23 | 28       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD21 | 28       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD22 | 28       | 0.24          |
| (1,652)  | 1:49:A:LEU:HD23 | 1:84:A:LEU:HD23 | 28       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 22       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 22       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 22       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 25       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 25       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 25       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 45       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 45       | 0.24          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 45       | 0.24          |
| (1,463)  | 1:49:A:LEU:HD11 | 1:55:A:GLY:H    | 49       | 0.24          |
| (1,463)  | 1:49:A:LEU:HD12 | 1:55:A:GLY:H    | 49       | 0.24          |
| (1,463)  | 1:49:A:LEU:HD13 | 1:55:A:GLY:H    | 49       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 23       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 23       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 23       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 23       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 23       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 23       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 23       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 23       | 0.24          |
| (1,438)  | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 23       | 0.24          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 8        | 0.24          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 8        | 0.24          |
| (1,424)  | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 8        | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 8        | 0.24          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 8        | 0.24          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 8        | 0.24          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 8        | 0.24          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 8        | 0.24          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 8        | 0.24          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 24       | 0.24          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 24       | 0.24          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 24       | 0.24          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 24       | 0.24          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 24       | 0.24          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 24       | 0.24          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 24       | 0.24          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 24       | 0.24          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 24       | 0.24          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 22       | 0.24          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 22       | 0.24          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 22       | 0.24          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 22       | 0.24          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 22       | 0.24          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 22       | 0.24          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 22       | 0.24          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 22       | 0.24          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 22       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 23       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 23       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 23       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 33       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 33       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 33       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 39       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 39       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 39       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 42       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 42       | 0.24          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 42       | 0.24          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 27       | 0.24          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 27       | 0.24          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 27       | 0.24          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 16       | 0.24          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 16       | 0.24          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 16       | 0.24          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 16       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 16       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 16       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 16       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 16       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 16       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 19       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 19       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 19       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 19       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 19       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 19       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 19       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 19       | 0.24          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 19       | 0.24          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 50       | 0.24          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 50       | 0.24          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 50       | 0.24          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 50       | 0.24          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 50       | 0.24          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 50       | 0.24          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 50       | 0.24          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 50       | 0.24          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 50       | 0.24          |
| (1,1779) | 1:75:A:LYS:HG2  | 1:79:A:ARG:HB2  | 18       | 0.23          |
| (1,1779) | 1:75:A:LYS:HG2  | 1:79:A:ARG:HB3  | 18       | 0.23          |
| (1,1779) | 1:75:A:LYS:HG3  | 1:79:A:ARG:HB2  | 18       | 0.23          |
| (1,1779) | 1:75:A:LYS:HG3  | 1:79:A:ARG:HB3  | 18       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 29       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 29       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 42       | 0.23          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 42       | 0.23          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 39       | 0.23          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 39       | 0.23          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 39       | 0.23          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 39       | 0.23          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 39       | 0.23          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 39       | 0.23          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 41       | 0.23          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 42       | 0.23          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 45       | 0.23          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 43       | 0.23          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 43       | 0.23          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 43       | 0.23          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 16       | 0.23          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 16       | 0.23          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 16       | 0.23          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 49       | 0.23          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 49       | 0.23          |
| (1,565)  | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 49       | 0.23          |
| (1,474)  | 1:49:A:LEU:HD21 | 1:81:A:TRP:HD1  | 28       | 0.23          |
| (1,474)  | 1:49:A:LEU:HD22 | 1:81:A:TRP:HD1  | 28       | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,474) | 1:49:A:LEU:HD23 | 1:81:A:TRP:HD1  | 28       | 0.23          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 34       | 0.23          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 34       | 0.23          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 34       | 0.23          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 34       | 0.23          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 34       | 0.23          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 34       | 0.23          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 34       | 0.23          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 34       | 0.23          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 34       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 16       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 31       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 39       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 44       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 44       | 0.23          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 44       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 44       | 0.23          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 44       | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 44       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 44       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 44       | 0.23          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 44       | 0.23          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 29       | 0.23          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 32       | 0.23          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 32       | 0.23          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 32       | 0.23          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 32       | 0.23          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 32       | 0.23          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 32       | 0.23          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 32       | 0.23          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 32       | 0.23          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 32       | 0.23          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 4        | 0.23          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 4        | 0.23          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 4        | 0.23          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 14       | 0.23          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 14       | 0.23          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 14       | 0.23          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 38       | 0.23          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 38       | 0.23          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 38       | 0.23          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 43       | 0.23          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 43       | 0.23          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 43       | 0.23          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 14       | 0.23          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 14       | 0.23          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 14       | 0.23          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 19       | 0.23          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 19       | 0.23          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 19       | 0.23          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 44       | 0.23          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 44       | 0.23          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 44       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 18       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 18       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 18       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 18       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 18       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 18       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 18       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 18       | 0.23          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 18       | 0.23          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 4        | 0.23          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 4        | 0.23          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 4        | 0.23          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 33       | 0.23          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 33       | 0.23          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 33       | 0.23          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 42       | 0.23          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 42       | 0.23          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 42       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 20       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 20       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 20       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 20       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 20       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 20       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 20       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 20       | 0.23          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 20       | 0.23          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 43       | 0.22          |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 43       | 0.22          |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 43       | 0.22          |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 43       | 0.22          |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 43       | 0.22          |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 43       | 0.22          |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 42       | 0.22          |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 42       | 0.22          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 48       | 0.22          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 48       | 0.22          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 48       | 0.22          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 48       | 0.22          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 48       | 0.22          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 48       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1488) | 1:35:A:VAL:HG11 | 1:39:A:LEU:HG   | 20       | 0.22          |
| (1,1488) | 1:35:A:VAL:HG12 | 1:39:A:LEU:HG   | 20       | 0.22          |
| (1,1488) | 1:35:A:VAL:HG13 | 1:39:A:LEU:HG   | 20       | 0.22          |
| (1,1488) | 1:35:A:VAL:HG21 | 1:39:A:LEU:HG   | 20       | 0.22          |
| (1,1488) | 1:35:A:VAL:HG22 | 1:39:A:LEU:HG   | 20       | 0.22          |
| (1,1488) | 1:35:A:VAL:HG23 | 1:39:A:LEU:HG   | 20       | 0.22          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 48       | 0.22          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 48       | 0.22          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 42       | 0.22          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 42       | 0.22          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 42       | 0.22          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 42       | 0.22          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 42       | 0.22          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 42       | 0.22          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 38       | 0.22          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 38       | 0.22          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 38       | 0.22          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 38       | 0.22          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 38       | 0.22          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 38       | 0.22          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 45       | 0.22          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 45       | 0.22          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 45       | 0.22          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 26       | 0.22          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 25       | 0.22          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 25       | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 25       | 0.22          |
| (1,934) | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 39       | 0.22          |
| (1,934) | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 39       | 0.22          |
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 39       | 0.22          |
| (1,934) | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 44       | 0.22          |
| (1,934) | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 44       | 0.22          |
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 44       | 0.22          |
| (1,625) | 1:65:A:THR:HG21 | 1:70:A:LEU:HD11 | 11       | 0.22          |
| (1,625) | 1:65:A:THR:HG21 | 1:70:A:LEU:HD12 | 11       | 0.22          |
| (1,625) | 1:65:A:THR:HG21 | 1:70:A:LEU:HD13 | 11       | 0.22          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD11 | 11       | 0.22          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD12 | 11       | 0.22          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD13 | 11       | 0.22          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD11 | 11       | 0.22          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD12 | 11       | 0.22          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD13 | 11       | 0.22          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD11 | 21       | 0.22          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD12 | 21       | 0.22          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD13 | 21       | 0.22          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 8        | 0.22          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 8        | 0.22          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 8        | 0.22          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 39       | 0.22          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 39       | 0.22          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 39       | 0.22          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 39       | 0.22          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 39       | 0.22          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 39       | 0.22          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 39       | 0.22          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 39       | 0.22          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 39       | 0.22          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 25       | 0.22          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 25       | 0.22          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 25       | 0.22          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 25       | 0.22          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 25       | 0.22          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 25       | 0.22          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 25       | 0.22          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 25       | 0.22          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 25       | 0.22          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 18       | 0.22          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 18       | 0.22          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 18       | 0.22          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 42       | 0.22          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 42       | 0.22          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 42       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 31       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 31       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 31       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 31       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 31       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 31       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 31       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 31       | 0.22          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 31       | 0.22          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 2        | 0.22          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 2        | 0.22          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 2        | 0.22          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 2        | 0.22          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 2        | 0.22          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 2        | 0.22          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 2        | 0.22          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 2        | 0.22          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 2        | 0.22          |
| (1,1608) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HG21 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HG22 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HG23 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HG21 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HG22 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HG23 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HG21 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HG22 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HG23 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD21 | 1:85:A:ILE:HG21 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD21 | 1:85:A:ILE:HG22 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD21 | 1:85:A:ILE:HG23 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD22 | 1:85:A:ILE:HG21 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD22 | 1:85:A:ILE:HG22 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD22 | 1:85:A:ILE:HG23 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD23 | 1:85:A:ILE:HG21 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD23 | 1:85:A:ILE:HG22 | 25       | 0.21          |
| (1,1608) | 1:49:A:LEU:HD23 | 1:85:A:ILE:HG23 | 25       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD11 | 1:70:A:LEU:HD11 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD11 | 1:70:A:LEU:HD12 | 45       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1505) | 1:36:A:ILE:HD11 | 1:70:A:LEU:HD13 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD11 | 1:70:A:LEU:HD21 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD11 | 1:70:A:LEU:HD22 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD11 | 1:70:A:LEU:HD23 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD12 | 1:70:A:LEU:HD11 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD12 | 1:70:A:LEU:HD12 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD12 | 1:70:A:LEU:HD13 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD12 | 1:70:A:LEU:HD21 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD12 | 1:70:A:LEU:HD22 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD12 | 1:70:A:LEU:HD23 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD13 | 1:70:A:LEU:HD11 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD13 | 1:70:A:LEU:HD12 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD13 | 1:70:A:LEU:HD13 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD13 | 1:70:A:LEU:HD21 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD13 | 1:70:A:LEU:HD22 | 45       | 0.21          |
| (1,1505) | 1:36:A:ILE:HD13 | 1:70:A:LEU:HD23 | 45       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD11 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD12 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD13 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD21 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD22 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD23 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD11 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD12 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD13 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD21 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD22 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD23 | 2        | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD11 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD12 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD13 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD21 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD22 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD23 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD11 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD12 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD13 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD21 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD22 | 24       | 0.21          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD23 | 24       | 0.21          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 33       | 0.21          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 33       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,993) | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 33       | 0.21          |
| (1,993) | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 34       | 0.21          |
| (1,993) | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 34       | 0.21          |
| (1,993) | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 34       | 0.21          |
| (1,934) | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 27       | 0.21          |
| (1,934) | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 27       | 0.21          |
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 27       | 0.21          |
| (1,663) | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 18       | 0.21          |
| (1,663) | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 18       | 0.21          |
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 18       | 0.21          |
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 18       | 0.21          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 18       | 0.21          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 18       | 0.21          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG21 | 32       | 0.21          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG22 | 32       | 0.21          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG23 | 32       | 0.21          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 12       | 0.21          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 12       | 0.21          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 12       | 0.21          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 14       | 0.21          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 14       | 0.21          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 14       | 0.21          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 20       | 0.21          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 20       | 0.21          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 20       | 0.21          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 36       | 0.21          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 36       | 0.21          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 36       | 0.21          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 46       | 0.21          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 46       | 0.21          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 46       | 0.21          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 31       | 0.21          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 44       | 0.21          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 44       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 44       | 0.21          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 44       | 0.21          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 44       | 0.21          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 44       | 0.21          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 44       | 0.21          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 44       | 0.21          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 44       | 0.21          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 1        | 0.21          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 2        | 0.21          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 2        | 0.21          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 2        | 0.21          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 2        | 0.21          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 2        | 0.21          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 2        | 0.21          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 2        | 0.21          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 2        | 0.21          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 2        | 0.21          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 8        | 0.21          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 8        | 0.21          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 8        | 0.21          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 8        | 0.21          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 8        | 0.21          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 8        | 0.21          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 8        | 0.21          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 8        | 0.21          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 8        | 0.21          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 41       | 0.21          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 41       | 0.21          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 41       | 0.21          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 46       | 0.21          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 46       | 0.21          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 46       | 0.21          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 35       | 0.21          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 35       | 0.21          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 35       | 0.21          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 46       | 0.21          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 46       | 0.21          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 46       | 0.21          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 29       | 0.21          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 29       | 0.21          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 29       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 42       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 42       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 42       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 42       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 42       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 42       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 42       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 42       | 0.21          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 42       | 0.21          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 39       | 0.21          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 39       | 0.21          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 39       | 0.21          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 39       | 0.21          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 39       | 0.21          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 39       | 0.21          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 39       | 0.21          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 39       | 0.21          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 39       | 0.21          |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 32       | 0.2           |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 32       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 6        | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 6        | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 15       | 0.2           |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 15       | 0.2           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 43       | 0.2           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 43       | 0.2           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 43       | 0.2           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 43       | 0.2           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 43       | 0.2           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 43       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG11 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG12 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG13 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG21 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG22 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG12 | 1:32:A:VAL:HG23 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG11 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG12 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG13 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG21 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG22 | 36       | 0.2           |
| (1,1418) | 1:26:A:ILE:HG13 | 1:32:A:VAL:HG23 | 36       | 0.2           |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 34       | 0.2           |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 34       | 0.2           |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 34       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 34       | 0.2           |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 34       | 0.2           |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 34       | 0.2           |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 50       | 0.2           |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 50       | 0.2           |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 50       | 0.2           |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 50       | 0.2           |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 50       | 0.2           |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 50       | 0.2           |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 19       | 0.2           |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 32       | 0.2           |
| (1,1067) | 1:49:A:LEU:HD11 | 1:54:A:LEU:H    | 34       | 0.2           |
| (1,1067) | 1:49:A:LEU:HD12 | 1:54:A:LEU:H    | 34       | 0.2           |
| (1,1067) | 1:49:A:LEU:HD13 | 1:54:A:LEU:H    | 34       | 0.2           |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 38       | 0.2           |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 43       | 0.2           |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 2        | 0.2           |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 2        | 0.2           |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 2        | 0.2           |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 24       | 0.2           |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 24       | 0.2           |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 24       | 0.2           |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 9        | 0.2           |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 9        | 0.2           |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 9        | 0.2           |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 9        | 0.2           |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 9        | 0.2           |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 9        | 0.2           |
| (1,630)  | 1:63:A:LYS:HA   | 1:65:A:THR:HG21 | 48       | 0.2           |
| (1,630)  | 1:63:A:LYS:HA   | 1:65:A:THR:HG22 | 48       | 0.2           |
| (1,630)  | 1:63:A:LYS:HA   | 1:65:A:THR:HG23 | 48       | 0.2           |
| (1,617)  | 1:60:A:ASP:HA   | 1:63:A:LYS:HB2  | 44       | 0.2           |
| (1,617)  | 1:60:A:ASP:HA   | 1:63:A:LYS:HB3  | 44       | 0.2           |
| (1,482)  | 1:10:A:GLN:HG2  | 1:52:A:THR:HG21 | 21       | 0.2           |
| (1,482)  | 1:10:A:GLN:HG2  | 1:52:A:THR:HG22 | 21       | 0.2           |
| (1,482)  | 1:10:A:GLN:HG2  | 1:52:A:THR:HG23 | 21       | 0.2           |
| (1,451)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 41       | 0.2           |
| (1,451)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 41       | 0.2           |
| (1,451)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 41       | 0.2           |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 4        | 0.2           |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 4        | 0.2           |
| (1,438)  | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 4        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 4        | 0.2           |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 4        | 0.2           |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 4        | 0.2           |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 4        | 0.2           |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 4        | 0.2           |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 4        | 0.2           |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 48       | 0.2           |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 48       | 0.2           |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 48       | 0.2           |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 48       | 0.2           |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 48       | 0.2           |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 48       | 0.2           |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 48       | 0.2           |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 48       | 0.2           |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 48       | 0.2           |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 33       | 0.2           |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 33       | 0.2           |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 33       | 0.2           |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 33       | 0.2           |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 33       | 0.2           |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 33       | 0.2           |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 33       | 0.2           |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 33       | 0.2           |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 33       | 0.2           |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 11       | 0.2           |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 11       | 0.2           |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 11       | 0.2           |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 11       | 0.2           |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 11       | 0.2           |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 11       | 0.2           |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 11       | 0.2           |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 11       | 0.2           |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 11       | 0.2           |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 13       | 0.2           |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 13       | 0.2           |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 13       | 0.2           |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 13       | 0.2           |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 13       | 0.2           |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 13       | 0.2           |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 13       | 0.2           |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 13       | 0.2           |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 13       | 0.2           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 27       | 0.2           |
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 27       | 0.2           |
| (1,423)  | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 27       | 0.2           |
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 27       | 0.2           |
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 27       | 0.2           |
| (1,423)  | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 27       | 0.2           |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 27       | 0.2           |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 27       | 0.2           |
| (1,423)  | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 27       | 0.2           |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 13       | 0.2           |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 13       | 0.2           |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 13       | 0.2           |
| (1,414)  | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 20       | 0.2           |
| (1,414)  | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 20       | 0.2           |
| (1,414)  | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 20       | 0.2           |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 17       | 0.2           |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 17       | 0.2           |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 17       | 0.2           |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 5        | 0.2           |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 5        | 0.2           |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 5        | 0.2           |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 12       | 0.2           |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 12       | 0.2           |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 12       | 0.2           |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 37       | 0.2           |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 37       | 0.2           |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 37       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 39       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 39       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 39       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 39       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 39       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 39       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 39       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 39       | 0.2           |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 39       | 0.2           |
| (1,379)  | 1:44:A:ILE:HB   | 1:81:A:TRP:HE1  | 38       | 0.2           |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 28       | 0.19          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 28       | 0.19          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 28       | 0.19          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 28       | 0.19          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 28       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 28       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB2  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB3  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB2  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB3  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB2  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB3  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB2  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB3  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB2  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB3  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB2  | 42       | 0.19          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB3  | 42       | 0.19          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG11 | 33       | 0.19          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG12 | 33       | 0.19          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG13 | 33       | 0.19          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG21 | 33       | 0.19          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG22 | 33       | 0.19          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG23 | 33       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 2        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 5        | 0.19          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD23 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD11 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD12 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD13 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD21 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD22 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD23 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD11 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD12 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD13 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD21 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD22 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD23 | 5        | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD11 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD12 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD13 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD21 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD22 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD23 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD11 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD12 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD13 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD21 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD22 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD23 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD11 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD12 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD13 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD21 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD22 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD23 | 12       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD11 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD12 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD13 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD21 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD22 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD23 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD11 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD12 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD13 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD21 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD22 | 37       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 37       | 0.19          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 37       | 0.19          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD11 | 22       | 0.19          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD12 | 22       | 0.19          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD13 | 22       | 0.19          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD21 | 22       | 0.19          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD22 | 22       | 0.19          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD23 | 22       | 0.19          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 35       | 0.19          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 35       | 0.19          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 35       | 0.19          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 35       | 0.19          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 35       | 0.19          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 35       | 0.19          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 49       | 0.19          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 49       | 0.19          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 49       | 0.19          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 49       | 0.19          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 49       | 0.19          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 49       | 0.19          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 44       | 0.19          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 44       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 44       | 0.19          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 48       | 0.19          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 48       | 0.19          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 48       | 0.19          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 48       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 48       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 48       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 48       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 48       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 48       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 48       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 50       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 50       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 50       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 50       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 50       | 0.19          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 50       | 0.19          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 27       | 0.19          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 27       | 0.19          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 27       | 0.19          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 27       | 0.19          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 27       | 0.19          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 27       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD11 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD12 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD13 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD21 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD22 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD23 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD11 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD12 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD13 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD21 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD22 | 36       | 0.19          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD23 | 36       | 0.19          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 39       | 0.19          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 48       | 0.19          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 48       | 0.19          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 48       | 0.19          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 41       | 0.19          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 41       | 0.19          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 41       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,934) | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 37       | 0.19          |
| (1,934) | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 37       | 0.19          |
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 37       | 0.19          |
| (1,873) | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 27       | 0.19          |
| (1,873) | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 47       | 0.19          |
| (1,625) | 1:65:A:THR:HG21 | 1:70:A:LEU:HD11 | 7        | 0.19          |
| (1,625) | 1:65:A:THR:HG21 | 1:70:A:LEU:HD12 | 7        | 0.19          |
| (1,625) | 1:65:A:THR:HG21 | 1:70:A:LEU:HD13 | 7        | 0.19          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD11 | 7        | 0.19          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD12 | 7        | 0.19          |
| (1,625) | 1:65:A:THR:HG22 | 1:70:A:LEU:HD13 | 7        | 0.19          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD11 | 7        | 0.19          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD12 | 7        | 0.19          |
| (1,625) | 1:65:A:THR:HG23 | 1:70:A:LEU:HD13 | 7        | 0.19          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD11 | 26       | 0.19          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD12 | 26       | 0.19          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD13 | 26       | 0.19          |
| (1,500) | 1:49:A:LEU:HD11 | 1:54:A:LEU:HB2  | 43       | 0.19          |
| (1,500) | 1:49:A:LEU:HD12 | 1:54:A:LEU:HB2  | 43       | 0.19          |
| (1,500) | 1:49:A:LEU:HD13 | 1:54:A:LEU:HB2  | 43       | 0.19          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD21 | 38       | 0.19          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD22 | 38       | 0.19          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD23 | 38       | 0.19          |
| (1,463) | 1:49:A:LEU:HD11 | 1:55:A:GLY:H    | 26       | 0.19          |
| (1,463) | 1:49:A:LEU:HD12 | 1:55:A:GLY:H    | 26       | 0.19          |
| (1,463) | 1:49:A:LEU:HD13 | 1:55:A:GLY:H    | 26       | 0.19          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 28       | 0.19          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 38       | 0.19          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 38       | 0.19          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 38       | 0.19          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 38       | 0.19          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 38       | 0.19          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 38       | 0.19          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 38       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 38       | 0.19          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 38       | 0.19          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 14       | 0.19          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 26       | 0.19          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 26       | 0.19          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 26       | 0.19          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 26       | 0.19          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 26       | 0.19          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 26       | 0.19          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 26       | 0.19          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 26       | 0.19          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 26       | 0.19          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 2        | 0.19          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 2        | 0.19          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 2        | 0.19          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 11       | 0.19          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 11       | 0.19          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 11       | 0.19          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 32       | 0.19          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 32       | 0.19          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 32       | 0.19          |
| (1,411) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HD21 | 38       | 0.19          |
| (1,411) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HD22 | 38       | 0.19          |
| (1,411) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HD23 | 38       | 0.19          |
| (1,411) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HD21 | 38       | 0.19          |
| (1,411) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HD22 | 38       | 0.19          |
| (1,411) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HD23 | 38       | 0.19          |
| (1,411) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HD21 | 38       | 0.19          |
| (1,411) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HD22 | 38       | 0.19          |
| (1,411) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HD23 | 38       | 0.19          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 47       | 0.19          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 47       | 0.19          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 47       | 0.19          |
| (1,407) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 47       | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 47       | 0.19          |
| (1,407)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 47       | 0.19          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 47       | 0.19          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 47       | 0.19          |
| (1,407)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 47       | 0.19          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 23       | 0.19          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 23       | 0.19          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 23       | 0.19          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 26       | 0.19          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 26       | 0.19          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 26       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 45       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 50       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 50       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 50       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 50       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 50       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 50       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 50       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 50       | 0.19          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 50       | 0.19          |
| (1,154)  | 1:20:A:ILE:HG21 | 1:29:A:MET:HA   | 47       | 0.19          |
| (1,154)  | 1:20:A:ILE:HG22 | 1:29:A:MET:HA   | 47       | 0.19          |
| (1,154)  | 1:20:A:ILE:HG23 | 1:29:A:MET:HA   | 47       | 0.19          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 2        | 0.18          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 2        | 0.18          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 2        | 0.18          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 2        | 0.18          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 2        | 0.18          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 2        | 0.18          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB2  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB3  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB2  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB3  | 38       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB2  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB3  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB2  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB3  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB2  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB3  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB2  | 38       | 0.18          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB3  | 38       | 0.18          |
| (1,1737) | 1:68:A:GLU:HG2  | 1:69:A:GLU:H    | 27       | 0.18          |
| (1,1737) | 1:68:A:GLU:HG3  | 1:69:A:GLU:H    | 27       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HB2  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HB3  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HB2  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HB3  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HB2  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HB3  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HB2  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD21 | 1:84:A:LEU:HB3  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HB2  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD22 | 1:84:A:LEU:HB3  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HB2  | 24       | 0.18          |
| (1,1605) | 1:49:A:LEU:HD23 | 1:84:A:LEU:HB3  | 24       | 0.18          |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 17       | 0.18          |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 17       | 0.18          |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 40       | 0.18          |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 40       | 0.18          |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 45       | 0.18          |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 45       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 1        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 1        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 9        | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 36       | 0.18          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 36       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 12       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 12       | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 12       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 12       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 12       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 12       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 18       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 18       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 18       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 18       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 18       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 18       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 35       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 35       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 35       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 35       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 35       | 0.18          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 35       | 0.18          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD11 | 34       | 0.18          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD12 | 34       | 0.18          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD13 | 34       | 0.18          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD11 | 34       | 0.18          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD12 | 34       | 0.18          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD13 | 34       | 0.18          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 8        | 0.18          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 8        | 0.18          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 8        | 0.18          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 8        | 0.18          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 8        | 0.18          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 8        | 0.18          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 25       | 0.18          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 25       | 0.18          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 25       | 0.18          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 25       | 0.18          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 25       | 0.18          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 25       | 0.18          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 25       | 0.18          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 49       | 0.18          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 49       | 0.18          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 49       | 0.18          |
| (1,1063) | 1:54:A:LEU:H    | 1:57:A:LEU:HG   | 26       | 0.18          |
| (1,701)  | 1:74:A:ALA:HA   | 1:77:A:LEU:HB3  | 41       | 0.18          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD11 | 43       | 0.18          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD12 | 43       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD13 | 43       | 0.18          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 11       | 0.18          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 11       | 0.18          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 11       | 0.18          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 21       | 0.18          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 21       | 0.18          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 21       | 0.18          |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD2  | 17       | 0.18          |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD3  | 17       | 0.18          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD21 | 50       | 0.18          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD22 | 50       | 0.18          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD23 | 50       | 0.18          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD11 | 48       | 0.18          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD12 | 48       | 0.18          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD13 | 48       | 0.18          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD11 | 48       | 0.18          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD12 | 48       | 0.18          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD13 | 48       | 0.18          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD11 | 48       | 0.18          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD12 | 48       | 0.18          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD13 | 48       | 0.18          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 3        | 0.18          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 22       | 0.18          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 22       | 0.18          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 22       | 0.18          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 22       | 0.18          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 22       | 0.18          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 22       | 0.18          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 22       | 0.18          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 22       | 0.18          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 22       | 0.18          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 16       | 0.18          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 16       | 0.18          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 16       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 22       | 0.18          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 22       | 0.18          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 22       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 14       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 14       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 14       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 27       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 27       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 27       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 44       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 44       | 0.18          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 44       | 0.18          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 7        | 0.18          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 7        | 0.18          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 7        | 0.18          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD21 | 24       | 0.18          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD22 | 24       | 0.18          |
| (1,407) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HD23 | 24       | 0.18          |
| (1,407) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD21 | 24       | 0.18          |
| (1,407) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD22 | 24       | 0.18          |
| (1,407) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HD23 | 24       | 0.18          |
| (1,407) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD21 | 24       | 0.18          |
| (1,407) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD22 | 24       | 0.18          |
| (1,407) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HD23 | 24       | 0.18          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 21       | 0.18          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 21       | 0.18          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 21       | 0.18          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 21       | 0.18          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 21       | 0.18          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 21       | 0.18          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 21       | 0.18          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 21       | 0.18          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 21       | 0.18          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 5        | 0.18          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 5        | 0.18          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 5        | 0.18          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 5        | 0.18          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 5        | 0.18          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 5        | 0.18          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 5        | 0.18          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 5        | 0.18          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 5        | 0.18          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 13       | 0.18          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 13       | 0.18          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 13       | 0.18          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 13       | 0.18          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 13       | 0.18          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 13       | 0.18          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 13       | 0.18          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 13       | 0.18          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 13       | 0.18          |
| (1,154)  | 1:20:A:ILE:HG21 | 1:29:A:MET:HA   | 33       | 0.18          |
| (1,154)  | 1:20:A:ILE:HG22 | 1:29:A:MET:HA   | 33       | 0.18          |
| (1,154)  | 1:20:A:ILE:HG23 | 1:29:A:MET:HA   | 33       | 0.18          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 42       | 0.17          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 42       | 0.17          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 42       | 0.17          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 42       | 0.17          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 42       | 0.17          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 42       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB2  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB3  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB2  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB3  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB2  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB3  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB2  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB3  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB2  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB3  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB2  | 28       | 0.17          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB3  | 28       | 0.17          |
| (1,1737) | 1:68:A:GLU:HG2  | 1:69:A:GLU:H    | 32       | 0.17          |
| (1,1737) | 1:68:A:GLU:HG3  | 1:69:A:GLU:H    | 32       | 0.17          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 50       | 0.17          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 50       | 0.17          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 50       | 0.17          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 50       | 0.17          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 50       | 0.17          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 50       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 8        | 0.17          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 8        | 0.17          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 8        | 0.17          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 8        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 8        | 0.17          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 8        | 0.17          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 20       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 20       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 20       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 20       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 20       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 20       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 50       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 50       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 50       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 50       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 50       | 0.17          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 50       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG11 | 1:36:A:ILE:HD11 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG11 | 1:36:A:ILE:HD12 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG11 | 1:36:A:ILE:HD13 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG12 | 1:36:A:ILE:HD11 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG12 | 1:36:A:ILE:HD12 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG12 | 1:36:A:ILE:HD13 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG13 | 1:36:A:ILE:HD11 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG13 | 1:36:A:ILE:HD12 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG13 | 1:36:A:ILE:HD13 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG21 | 1:36:A:ILE:HD11 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG21 | 1:36:A:ILE:HD12 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG21 | 1:36:A:ILE:HD13 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG22 | 1:36:A:ILE:HD11 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG22 | 1:36:A:ILE:HD12 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG22 | 1:36:A:ILE:HD13 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG23 | 1:36:A:ILE:HD11 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG23 | 1:36:A:ILE:HD12 | 45       | 0.17          |
| (1,1462) | 1:32:A:VAL:HG23 | 1:36:A:ILE:HD13 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 42       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 42       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 45       | 0.17          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 45       | 0.17          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 23       | 0.17          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 23       | 0.17          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 23       | 0.17          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 23       | 0.17          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 23       | 0.17          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 23       | 0.17          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 23       | 0.17          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 23       | 0.17          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 23       | 0.17          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 23       | 0.17          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD11 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD12 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD13 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD21 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD22 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD23 | 4        | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD11 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD12 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD13 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD21 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD22 | 4        | 0.17          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD23 | 4        | 0.17          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 31       | 0.17          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 18       | 0.17          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 18       | 0.17          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 18       | 0.17          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 42       | 0.17          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 42       | 0.17          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 42       | 0.17          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 44       | 0.17          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 26       | 0.17          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 26       | 0.17          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 26       | 0.17          |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE2  | 38       | 0.17          |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE3  | 38       | 0.17          |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE2  | 45       | 0.17          |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE3  | 45       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD11 | 41       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD12 | 41       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD13 | 41       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD11 | 41       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD12 | 41       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD13 | 41       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD11 | 41       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD12 | 41       | 0.17          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD13 | 41       | 0.17          |
| (1,678)  | 1:62:A:ARG:HG2  | 1:74:A:ALA:HB1  | 43       | 0.17          |
| (1,678)  | 1:62:A:ARG:HG2  | 1:74:A:ALA:HB2  | 43       | 0.17          |
| (1,678)  | 1:62:A:ARG:HG2  | 1:74:A:ALA:HB3  | 43       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 29       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 29       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 29       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 29       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 29       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 29       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 32       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 32       | 0.17          |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 32       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 32       | 0.17          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 32       | 0.17          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 32       | 0.17          |
| (1,663) | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 34       | 0.17          |
| (1,663) | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 34       | 0.17          |
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 34       | 0.17          |
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 34       | 0.17          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 34       | 0.17          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 34       | 0.17          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG21 | 28       | 0.17          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG22 | 28       | 0.17          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG23 | 28       | 0.17          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG21 | 49       | 0.17          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG22 | 49       | 0.17          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG23 | 49       | 0.17          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 9        | 0.17          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 9        | 0.17          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 9        | 0.17          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 32       | 0.17          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 32       | 0.17          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 32       | 0.17          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 33       | 0.17          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 33       | 0.17          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 33       | 0.17          |
| (1,455) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD21 | 36       | 0.17          |
| (1,455) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD22 | 36       | 0.17          |
| (1,455) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD23 | 36       | 0.17          |
| (1,455) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD21 | 36       | 0.17          |
| (1,455) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD22 | 36       | 0.17          |
| (1,455) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD23 | 36       | 0.17          |
| (1,455) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD21 | 36       | 0.17          |
| (1,455) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD22 | 36       | 0.17          |
| (1,455) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD23 | 36       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 16       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 16       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 16       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 16       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 16       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 16       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 16       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 16       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 16       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 19       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 21       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 29       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 29       | 0.17          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 29       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 29       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 29       | 0.17          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 29       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 29       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 29       | 0.17          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 29       | 0.17          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 8        | 0.17          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 22       | 0.17          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 22       | 0.17          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 22       | 0.17          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 22       | 0.17          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 22       | 0.17          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 22       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 22       | 0.17          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 22       | 0.17          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 22       | 0.17          |
| (1,427) | 1:45:A:THR:HG21 | 1:46:A:LYS:H    | 23       | 0.17          |
| (1,427) | 1:45:A:THR:HG22 | 1:46:A:LYS:H    | 23       | 0.17          |
| (1,427) | 1:45:A:THR:HG23 | 1:46:A:LYS:H    | 23       | 0.17          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 3        | 0.17          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 3        | 0.17          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 3        | 0.17          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 8        | 0.17          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 8        | 0.17          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 8        | 0.17          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 34       | 0.17          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 34       | 0.17          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 34       | 0.17          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD11 | 49       | 0.17          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD12 | 49       | 0.17          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD13 | 49       | 0.17          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 15       | 0.17          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 15       | 0.17          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 15       | 0.17          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 17       | 0.17          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 17       | 0.17          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 17       | 0.17          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 32       | 0.17          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 32       | 0.17          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 32       | 0.17          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 24       | 0.17          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 24       | 0.17          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 24       | 0.17          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 24       | 0.17          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 24       | 0.17          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 24       | 0.17          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 24       | 0.17          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 24       | 0.17          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 24       | 0.17          |
| (1,359) | 1:39:A:LEU:HA   | 1:42:A:TYR:HB3  | 50       | 0.17          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 16       | 0.17          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 16       | 0.17          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 16       | 0.17          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 16       | 0.17          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 16       | 0.17          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 16       | 0.17          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 16       | 0.17          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 16       | 0.17          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 16       | 0.17          |
| (1,154)  | 1:20:A:ILE:HG21 | 1:29:A:MET:HA   | 22       | 0.17          |
| (1,154)  | 1:20:A:ILE:HG22 | 1:29:A:MET:HA   | 22       | 0.17          |
| (1,154)  | 1:20:A:ILE:HG23 | 1:29:A:MET:HA   | 22       | 0.17          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 30       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 30       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 30       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 30       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 30       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 30       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 40       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 40       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 40       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 40       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 40       | 0.16          |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 40       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 36       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 36       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 36       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 36       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 36       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 36       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 48       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 48       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 48       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 48       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 48       | 0.16          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB2  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB3  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB2  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB3  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB2  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB3  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB2  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB3  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB2  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB3  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB2  | 20       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB3  | 20       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB2  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB3  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB2  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB3  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB2  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB3  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB2  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB3  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB2  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB3  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB2  | 48       | 0.16          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB3  | 48       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 22       | 0.16          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 22       | 0.16          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD11 | 49       | 0.16          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD12 | 49       | 0.16          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD13 | 49       | 0.16          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD21 | 49       | 0.16          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD22 | 49       | 0.16          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD23 | 49       | 0.16          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 39       | 0.16          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 39       | 0.16          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 39       | 0.16          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 39       | 0.16          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 39       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 39       | 0.16          |
| (1,1527) | 1:39:A:LEU:HD11 | 1:44:A:ILE:H    | 39       | 0.16          |
| (1,1527) | 1:39:A:LEU:HD12 | 1:44:A:ILE:H    | 39       | 0.16          |
| (1,1527) | 1:39:A:LEU:HD13 | 1:44:A:ILE:H    | 39       | 0.16          |
| (1,1527) | 1:39:A:LEU:HD21 | 1:44:A:ILE:H    | 39       | 0.16          |
| (1,1527) | 1:39:A:LEU:HD22 | 1:44:A:ILE:H    | 39       | 0.16          |
| (1,1527) | 1:39:A:LEU:HD23 | 1:44:A:ILE:H    | 39       | 0.16          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 11       | 0.16          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 11       | 0.16          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 11       | 0.16          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 11       | 0.16          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 11       | 0.16          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 11       | 0.16          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD11 | 33       | 0.16          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD12 | 33       | 0.16          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD13 | 33       | 0.16          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD11 | 33       | 0.16          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD12 | 33       | 0.16          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD13 | 33       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 17       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 17       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 17       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 17       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 17       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 17       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 19       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 19       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 19       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 19       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 19       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 19       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 41       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 41       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 41       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 41       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 41       | 0.16          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 41       | 0.16          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 29       | 0.16          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 33       | 0.16          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 50       | 0.16          |
| (1,663)  | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 50       | 0.16          |
| (1,663)  | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 50       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 50       | 0.16          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 50       | 0.16          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 50       | 0.16          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD11 | 27       | 0.16          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD12 | 27       | 0.16          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD13 | 27       | 0.16          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 10       | 0.16          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 10       | 0.16          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 10       | 0.16          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 18       | 0.16          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 18       | 0.16          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 18       | 0.16          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 32       | 0.16          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 32       | 0.16          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 2        | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 32       | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 35       | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 35       | 0.16          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 35       | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 35       | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 35       | 0.16          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 35       | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 35       | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 35       | 0.16          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 35       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,427) | 1:45:A:THR:HG21 | 1:46:A:LYS:H    | 21       | 0.16          |
| (1,427) | 1:45:A:THR:HG22 | 1:46:A:LYS:H    | 21       | 0.16          |
| (1,427) | 1:45:A:THR:HG23 | 1:46:A:LYS:H    | 21       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 3        | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 9        | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 24       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 35       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 37       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 37       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 37       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 37       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 37       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 37       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 37       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 37       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 37       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 38       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 41       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 50       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 50       | 0.16          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 50       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 50       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 50       | 0.16          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 50       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 50       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 50       | 0.16          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 50       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 24       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 24       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 24       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 26       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 26       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 26       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 47       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 47       | 0.16          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 47       | 0.16          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 49       | 0.16          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 49       | 0.16          |
| (1,413)  | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 49       | 0.16          |
| (1,410)  | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 20       | 0.16          |
| (1,410)  | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 20       | 0.16          |
| (1,410)  | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 20       | 0.16          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 35       | 0.16          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 35       | 0.16          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 35       | 0.16          |
| (1,402)  | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 39       | 0.16          |
| (1,402)  | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 39       | 0.16          |
| (1,402)  | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 39       | 0.16          |
| (1,359)  | 1:39:A:LEU:HA   | 1:42:A:TYR:HB3  | 27       | 0.16          |
| (1,359)  | 1:39:A:LEU:HA   | 1:42:A:TYR:HB3  | 45       | 0.16          |
| (1,335)  | 1:36:A:ILE:HG21 | 1:77:A:LEU:H    | 35       | 0.16          |
| (1,335)  | 1:36:A:ILE:HG22 | 1:77:A:LEU:H    | 35       | 0.16          |
| (1,335)  | 1:36:A:ILE:HG23 | 1:77:A:LEU:H    | 35       | 0.16          |
| (1,335)  | 1:36:A:ILE:HG21 | 1:77:A:LEU:H    | 37       | 0.16          |
| (1,335)  | 1:36:A:ILE:HG22 | 1:77:A:LEU:H    | 37       | 0.16          |
| (1,335)  | 1:36:A:ILE:HG23 | 1:77:A:LEU:H    | 37       | 0.16          |
| (1,259)  | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 48       | 0.16          |
| (1,259)  | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 48       | 0.16          |
| (1,259)  | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 48       | 0.16          |
| (1,259)  | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 48       | 0.16          |
| (1,259)  | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 48       | 0.16          |
| (1,259)  | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 48       | 0.16          |
| (1,259)  | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 48       | 0.16          |
| (1,259)  | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 48       | 0.16          |
| (1,259)  | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 48       | 0.16          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 49       | 0.16          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 49       | 0.16          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 49       | 0.16          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 49       | 0.16          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 49       | 0.16          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 49       | 0.16          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 49       | 0.16          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 49       | 0.16          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 49       | 0.16          |
| (1,192)  | 1:26:A:ILE:HD11 | 1:32:A:VAL:H    | 40       | 0.16          |
| (1,192)  | 1:26:A:ILE:HD12 | 1:32:A:VAL:H    | 40       | 0.16          |
| (1,192)  | 1:26:A:ILE:HD13 | 1:32:A:VAL:H    | 40       | 0.16          |
| (1,1805) | 1:78:A:LEU:HD11 | 1:81:A:TRP:HH2  | 32       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1805) | 1:78:A:LEU:HD12 | 1:81:A:TRP:HH2  | 32       | 0.15          |
| (1,1805) | 1:78:A:LEU:HD13 | 1:81:A:TRP:HH2  | 32       | 0.15          |
| (1,1805) | 1:78:A:LEU:HD21 | 1:81:A:TRP:HH2  | 32       | 0.15          |
| (1,1805) | 1:78:A:LEU:HD22 | 1:81:A:TRP:HH2  | 32       | 0.15          |
| (1,1805) | 1:78:A:LEU:HD23 | 1:81:A:TRP:HH2  | 32       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 17       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 17       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 17       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 17       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 17       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 17       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 20       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 20       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 20       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 20       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 20       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 20       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 27       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 34       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 34       | 0.15          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 34       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 17       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 17       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 17       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 17       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 17       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 17       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 30       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 30       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 30       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 30       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 30       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 30       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 39       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 39       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 39       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 39       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 39       | 0.15          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 39       | 0.15          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD11 | 31       | 0.15          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD12 | 31       | 0.15          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD13 | 31       | 0.15          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD21 | 31       | 0.15          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD22 | 31       | 0.15          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD23 | 31       | 0.15          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 27       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 27       | 0.15          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 27       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 22       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 22       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 22       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 22       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 22       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 22       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 47       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 47       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 47       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 47       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 47       | 0.15          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 47       | 0.15          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 25       | 0.15          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 25       | 0.15          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 25       | 0.15          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 25       | 0.15          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 25       | 0.15          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 25       | 0.15          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 46       | 0.15          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 30       | 0.15          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 30       | 0.15          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 30       | 0.15          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 34       | 0.15          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 34       | 0.15          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 34       | 0.15          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 4        | 0.15          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 4        | 0.15          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 4        | 0.15          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 21       | 0.15          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 21       | 0.15          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 21       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,993) | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 27       | 0.15          |
| (1,993) | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 27       | 0.15          |
| (1,993) | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 27       | 0.15          |
| (1,993) | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 44       | 0.15          |
| (1,993) | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 44       | 0.15          |
| (1,993) | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 44       | 0.15          |
| (1,934) | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 18       | 0.15          |
| (1,934) | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 18       | 0.15          |
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 18       | 0.15          |
| (1,934) | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 30       | 0.15          |
| (1,934) | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 30       | 0.15          |
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 30       | 0.15          |
| (1,934) | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 42       | 0.15          |
| (1,934) | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 42       | 0.15          |
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 42       | 0.15          |
| (1,934) | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 50       | 0.15          |
| (1,934) | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 50       | 0.15          |
| (1,934) | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 50       | 0.15          |
| (1,873) | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 32       | 0.15          |
| (1,873) | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 45       | 0.15          |
| (1,655) | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD21 | 28       | 0.15          |
| (1,655) | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD22 | 28       | 0.15          |
| (1,655) | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD23 | 28       | 0.15          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG21 | 19       | 0.15          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG22 | 19       | 0.15          |
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG23 | 19       | 0.15          |
| (1,617) | 1:60:A:ASP:HA   | 1:63:A:LYS:HB2  | 26       | 0.15          |
| (1,617) | 1:60:A:ASP:HA   | 1:63:A:LYS:HB3  | 26       | 0.15          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 2        | 0.15          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 2        | 0.15          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 2        | 0.15          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 3        | 0.15          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 3        | 0.15          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 3        | 0.15          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 42       | 0.15          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 42       | 0.15          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 42       | 0.15          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 28       | 0.15          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 28       | 0.15          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 28       | 0.15          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 37       | 0.15          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 37       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 37       | 0.15          |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD2  | 4        | 0.15          |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD3  | 4        | 0.15          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD11 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD12 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD13 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD11 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD12 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD13 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD11 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD12 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD13 | 12       | 0.15          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD11 | 16       | 0.15          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD12 | 16       | 0.15          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD13 | 16       | 0.15          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD11 | 16       | 0.15          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD12 | 16       | 0.15          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD13 | 16       | 0.15          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD11 | 16       | 0.15          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD12 | 16       | 0.15          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD13 | 16       | 0.15          |
| (1,451) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 33       | 0.15          |
| (1,451) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 33       | 0.15          |
| (1,451) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 33       | 0.15          |
| (1,451) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 40       | 0.15          |
| (1,451) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 40       | 0.15          |
| (1,451) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 40       | 0.15          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 42       | 0.15          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 42       | 0.15          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 42       | 0.15          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 42       | 0.15          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 42       | 0.15          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 42       | 0.15          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 42       | 0.15          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 42       | 0.15          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 42       | 0.15          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 10       | 0.15          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 10       | 0.15          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 10       | 0.15          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 10       | 0.15          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 10       | 0.15          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 10       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 10       | 0.15          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 10       | 0.15          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 10       | 0.15          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 21       | 0.15          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 21       | 0.15          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 21       | 0.15          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 21       | 0.15          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 21       | 0.15          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 21       | 0.15          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 21       | 0.15          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 21       | 0.15          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 21       | 0.15          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 34       | 0.15          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 34       | 0.15          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 34       | 0.15          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 34       | 0.15          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 34       | 0.15          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 34       | 0.15          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 34       | 0.15          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 34       | 0.15          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 34       | 0.15          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 12       | 0.15          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 12       | 0.15          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 12       | 0.15          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 21       | 0.15          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 21       | 0.15          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 21       | 0.15          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 1        | 0.15          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 1        | 0.15          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 1        | 0.15          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD11 | 26       | 0.15          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD12 | 26       | 0.15          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD13 | 26       | 0.15          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 8        | 0.15          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 8        | 0.15          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 8        | 0.15          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 18       | 0.15          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 18       | 0.15          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 18       | 0.15          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 28       | 0.15          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 28       | 0.15          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 28       | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 7        | 0.15          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 12       | 0.15          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 12       | 0.15          |
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 12       | 0.15          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 12       | 0.15          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 12       | 0.15          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 12       | 0.15          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 12       | 0.15          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 12       | 0.15          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 12       | 0.15          |
| (1,359)  | 1:39:A:LEU:HA   | 1:42:A:TYR:HB3  | 26       | 0.15          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 43       | 0.15          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 43       | 0.15          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 43       | 0.15          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 43       | 0.15          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 43       | 0.15          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 43       | 0.15          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 43       | 0.15          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 43       | 0.15          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 43       | 0.15          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 44       | 0.14          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 44       | 0.14          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 44       | 0.14          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 44       | 0.14          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 44       | 0.14          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 44       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB2  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB3  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB2  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB3  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB2  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB3  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB2  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB3  | 39       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB2  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB3  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB2  | 39       | 0.14          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB3  | 39       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 24       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 24       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 24       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 24       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 24       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 24       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 35       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 35       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 35       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 35       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 35       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 35       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 41       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 41       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 41       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 41       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 41       | 0.14          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 41       | 0.14          |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 37       | 0.14          |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 37       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 7        | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 7        | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD11 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD12 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD13 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD21 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD22 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD23 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD11 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD12 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD13 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD21 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD22 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD23 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD11 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD12 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD13 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD21 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD22 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD23 | 28       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD11 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD12 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD13 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD21 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD22 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD23 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD11 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD12 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD13 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD21 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD22 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD23 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD11 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD12 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD13 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD21 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD22 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD23 | 32       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD11 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD12 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD13 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD21 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD22 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB1 | 1:49:A:LEU:HD23 | 45       | 0.14          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD11 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD12 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD13 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD21 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD22 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB2 | 1:49:A:LEU:HD23 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD11 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD12 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD13 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD21 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD22 | 45       | 0.14          |
| (1,1582) | 1:48:A:ALA:HB3 | 1:49:A:LEU:HD23 | 45       | 0.14          |
| (1,1576) | 1:46:A:LYS:HB2 | 1:85:A:ILE:HG21 | 9        | 0.14          |
| (1,1576) | 1:46:A:LYS:HB2 | 1:85:A:ILE:HG22 | 9        | 0.14          |
| (1,1576) | 1:46:A:LYS:HB2 | 1:85:A:ILE:HG23 | 9        | 0.14          |
| (1,1576) | 1:46:A:LYS:HB3 | 1:85:A:ILE:HG21 | 9        | 0.14          |
| (1,1576) | 1:46:A:LYS:HB3 | 1:85:A:ILE:HG22 | 9        | 0.14          |
| (1,1576) | 1:46:A:LYS:HB3 | 1:85:A:ILE:HG23 | 9        | 0.14          |
| (1,1576) | 1:46:A:LYS:HB2 | 1:85:A:ILE:HG21 | 36       | 0.14          |
| (1,1576) | 1:46:A:LYS:HB2 | 1:85:A:ILE:HG22 | 36       | 0.14          |
| (1,1576) | 1:46:A:LYS:HB2 | 1:85:A:ILE:HG23 | 36       | 0.14          |
| (1,1576) | 1:46:A:LYS:HB3 | 1:85:A:ILE:HG21 | 36       | 0.14          |
| (1,1576) | 1:46:A:LYS:HB3 | 1:85:A:ILE:HG22 | 36       | 0.14          |
| (1,1576) | 1:46:A:LYS:HB3 | 1:85:A:ILE:HG23 | 36       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD11 | 9        | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD12 | 9        | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD13 | 9        | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD21 | 9        | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD22 | 9        | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD23 | 9        | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD11 | 13       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD12 | 13       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD13 | 13       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD21 | 13       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD22 | 13       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD23 | 13       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD11 | 28       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD12 | 28       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD13 | 28       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD21 | 28       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD22 | 28       | 0.14          |
| (1,1557) | 1:44:A:ILE:HB  | 1:49:A:LEU:HD23 | 28       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 16       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 16       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 16       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 16       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 16       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 16       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 47       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 47       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 47       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 47       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 47       | 0.14          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 47       | 0.14          |
| (1,1496) | 1:36:A:ILE:HG21 | 1:37:A:SER:HB2  | 42       | 0.14          |
| (1,1496) | 1:36:A:ILE:HG21 | 1:37:A:SER:HB3  | 42       | 0.14          |
| (1,1496) | 1:36:A:ILE:HG22 | 1:37:A:SER:HB2  | 42       | 0.14          |
| (1,1496) | 1:36:A:ILE:HG22 | 1:37:A:SER:HB3  | 42       | 0.14          |
| (1,1496) | 1:36:A:ILE:HG23 | 1:37:A:SER:HB2  | 42       | 0.14          |
| (1,1496) | 1:36:A:ILE:HG23 | 1:37:A:SER:HB3  | 42       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 19       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 38       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 38       | 0.14          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 38       | 0.14          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 24       | 0.14          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 24       | 0.14          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 24       | 0.14          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 24       | 0.14          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 2        | 0.14          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 2        | 0.14          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 2        | 0.14          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 2        | 0.14          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 2        | 0.14          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 2        | 0.14          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 44       | 0.14          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 44       | 0.14          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 44       | 0.14          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 44       | 0.14          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 44       | 0.14          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 44       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 26       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 26       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 26       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 26       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 26       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 26       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 29       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 29       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 29       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 29       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 29       | 0.14          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 29       | 0.14          |
| (1,1288) | 1:12:A:ILE:HG12 | 1:42:A:TYR:HB2  | 25       | 0.14          |
| (1,1288) | 1:12:A:ILE:HG12 | 1:42:A:TYR:HB3  | 25       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1288) | 1:12:A:ILE:HG13 | 1:42:A:TYR:HB2  | 25       | 0.14          |
| (1,1288) | 1:12:A:ILE:HG13 | 1:42:A:TYR:HB3  | 25       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 17       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 17       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 17       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 26       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 26       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 26       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 31       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 31       | 0.14          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 31       | 0.14          |
| (1,1067) | 1:49:A:LEU:HD11 | 1:54:A:LEU:H    | 3        | 0.14          |
| (1,1067) | 1:49:A:LEU:HD12 | 1:54:A:LEU:H    | 3        | 0.14          |
| (1,1067) | 1:49:A:LEU:HD13 | 1:54:A:LEU:H    | 3        | 0.14          |
| (1,1067) | 1:49:A:LEU:HD11 | 1:54:A:LEU:H    | 13       | 0.14          |
| (1,1067) | 1:49:A:LEU:HD12 | 1:54:A:LEU:H    | 13       | 0.14          |
| (1,1067) | 1:49:A:LEU:HD13 | 1:54:A:LEU:H    | 13       | 0.14          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 19       | 0.14          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 19       | 0.14          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 19       | 0.14          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 38       | 0.14          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 38       | 0.14          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 38       | 0.14          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 46       | 0.14          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 46       | 0.14          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 46       | 0.14          |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 41       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD11 | 37       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD12 | 37       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD13 | 37       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD11 | 37       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD12 | 37       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD13 | 37       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD11 | 37       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD12 | 37       | 0.14          |
| (1,749)  | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD13 | 37       | 0.14          |
| (1,617)  | 1:60:A:ASP:HA   | 1:63:A:LYS:HB2  | 45       | 0.14          |
| (1,617)  | 1:60:A:ASP:HA   | 1:63:A:LYS:HB3  | 45       | 0.14          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD11 | 45       | 0.14          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD12 | 45       | 0.14          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD13 | 45       | 0.14          |
| (1,601)  | 1:62:A:ARG:HA   | 1:70:A:LEU:HD11 | 48       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD12 | 48       | 0.14          |
| (1,601) | 1:62:A:ARG:HA   | 1:70:A:LEU:HD13 | 48       | 0.14          |
| (1,567) | 1:58:A:ILE:HD11 | 1:59:A:ASN:H    | 34       | 0.14          |
| (1,567) | 1:58:A:ILE:HD12 | 1:59:A:ASN:H    | 34       | 0.14          |
| (1,567) | 1:58:A:ILE:HD13 | 1:59:A:ASN:H    | 34       | 0.14          |
| (1,552) | 1:54:A:LEU:HB3  | 1:58:A:ILE:HD11 | 45       | 0.14          |
| (1,552) | 1:54:A:LEU:HB3  | 1:58:A:ILE:HD12 | 45       | 0.14          |
| (1,552) | 1:54:A:LEU:HB3  | 1:58:A:ILE:HD13 | 45       | 0.14          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 23       | 0.14          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 23       | 0.14          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 23       | 0.14          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 32       | 0.14          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 32       | 0.14          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 32       | 0.14          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 29       | 0.14          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 29       | 0.14          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 29       | 0.14          |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD2  | 2        | 0.14          |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD3  | 2        | 0.14          |
| (1,491) | 1:51:A:GLU:H    | 1:52:A:THR:HG21 | 32       | 0.14          |
| (1,491) | 1:51:A:GLU:H    | 1:52:A:THR:HG22 | 32       | 0.14          |
| (1,491) | 1:51:A:GLU:H    | 1:52:A:THR:HG23 | 32       | 0.14          |
| (1,474) | 1:49:A:LEU:HD21 | 1:81:A:TRP:HD1  | 43       | 0.14          |
| (1,474) | 1:49:A:LEU:HD22 | 1:81:A:TRP:HD1  | 43       | 0.14          |
| (1,474) | 1:49:A:LEU:HD23 | 1:81:A:TRP:HD1  | 43       | 0.14          |
| (1,451) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 42       | 0.14          |
| (1,451) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 42       | 0.14          |
| (1,451) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 42       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 5        | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 12       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 12       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 12       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 12       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 12       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 12       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 12       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 12       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 12       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 20       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 24       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 30       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 37       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 37       | 0.14          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 37       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 37       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 37       | 0.14          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 37       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 37       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 37       | 0.14          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 37       | 0.14          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 35       | 0.14          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 35       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 35       | 0.14          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 35       | 0.14          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 35       | 0.14          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 35       | 0.14          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 35       | 0.14          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 35       | 0.14          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 35       | 0.14          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 49       | 0.14          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 49       | 0.14          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 49       | 0.14          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 49       | 0.14          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 49       | 0.14          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 49       | 0.14          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 49       | 0.14          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 49       | 0.14          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 49       | 0.14          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG21 | 13       | 0.14          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG22 | 13       | 0.14          |
| (1,424) | 1:44:A:ILE:HD11 | 1:45:A:THR:HG23 | 13       | 0.14          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG21 | 13       | 0.14          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG22 | 13       | 0.14          |
| (1,424) | 1:44:A:ILE:HD12 | 1:45:A:THR:HG23 | 13       | 0.14          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG21 | 13       | 0.14          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG22 | 13       | 0.14          |
| (1,424) | 1:44:A:ILE:HD13 | 1:45:A:THR:HG23 | 13       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 11       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 19       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 19       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 19       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 19       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 19       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 19       | 0.14          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 19       | 0.14          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 19       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 19       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 46       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 46       | 0.14          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 46       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 46       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 46       | 0.14          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 46       | 0.14          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 46       | 0.14          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 46       | 0.14          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 46       | 0.14          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 1        | 0.14          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 1        | 0.14          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 1        | 0.14          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 15       | 0.14          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 15       | 0.14          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 15       | 0.14          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD11 | 45       | 0.14          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD12 | 45       | 0.14          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD13 | 45       | 0.14          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 19       | 0.14          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 19       | 0.14          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 19       | 0.14          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 47       | 0.14          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 47       | 0.14          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 47       | 0.14          |
| (1,259) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 44       | 0.14          |
| (1,259) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 44       | 0.14          |
| (1,259) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 44       | 0.14          |
| (1,259) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 44       | 0.14          |
| (1,259) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 44       | 0.14          |
| (1,259) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 44       | 0.14          |
| (1,259) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 44       | 0.14          |
| (1,259) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 44       | 0.14          |
| (1,259) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 44       | 0.14          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 27       | 0.14          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 27       | 0.14          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 27       | 0.14          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 27       | 0.14          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 27       | 0.14          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 27       | 0.14          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 27       | 0.14          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 27       | 0.14          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 27       | 0.14          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 42       | 0.14          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 42       | 0.14          |
| (1,224)  | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 42       | 0.14          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 42       | 0.14          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 42       | 0.14          |
| (1,224)  | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 42       | 0.14          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 42       | 0.14          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 42       | 0.14          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 42       | 0.14          |
| (1,169)  | 1:23:A:GLN:HB3  | 1:25:A:ASN:HD22 | 40       | 0.14          |
| (1,154)  | 1:20:A:ILE:HG21 | 1:29:A:MET:HA   | 31       | 0.14          |
| (1,154)  | 1:20:A:ILE:HG22 | 1:29:A:MET:HA   | 31       | 0.14          |
| (1,154)  | 1:20:A:ILE:HG23 | 1:29:A:MET:HA   | 31       | 0.14          |
| (1,154)  | 1:20:A:ILE:HG21 | 1:29:A:MET:HA   | 46       | 0.14          |
| (1,154)  | 1:20:A:ILE:HG22 | 1:29:A:MET:HA   | 46       | 0.14          |
| (1,154)  | 1:20:A:ILE:HG23 | 1:29:A:MET:HA   | 46       | 0.14          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD11 | 44       | 0.14          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD12 | 44       | 0.14          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD13 | 44       | 0.14          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 34       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 34       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 34       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 34       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 34       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 34       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 47       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 47       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 47       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 47       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 47       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 47       | 0.13          |
| (1,1737) | 1:68:A:GLU:HG2  | 1:69:A:GLU:H    | 28       | 0.13          |
| (1,1737) | 1:68:A:GLU:HG3  | 1:69:A:GLU:H    | 28       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 18       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 18       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 18       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 18       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 18       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 18       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 28       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 28       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 28       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 28       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 28       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 28       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 49       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 49       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 49       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 49       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 49       | 0.13          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 49       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 10       | 0.13          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 10       | 0.13          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 45       | 0.13          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 45       | 0.13          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 45       | 0.13          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 45       | 0.13          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 45       | 0.13          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 45       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 24       | 0.13          |

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| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG13 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG21 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG22 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG23 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG11 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG12 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG13 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG21 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG22 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG23 | 24       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG11 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG12 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG13 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG21 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG22 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG23 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG11 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG12 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG13 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG21 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG22 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG23 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG11 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG12 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG13 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG21 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG22 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG23 | 32       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG11 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG12 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG13 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG21 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG22 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG23 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG11 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG12 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG13 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG21 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG22 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG23 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG11 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG12 | 41       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 41       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG11 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG12 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG13 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG11 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG12 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG13 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG11 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG12 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG13 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 49       | 0.13          |
| (1,1435) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 49       | 0.13          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 30       | 0.13          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 30       | 0.13          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 30       | 0.13          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 30       | 0.13          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 35       | 0.13          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 35       | 0.13          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 35       | 0.13          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 35       | 0.13          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD11 | 17       | 0.13          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD12 | 17       | 0.13          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD13 | 17       | 0.13          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD11 | 17       | 0.13          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD12 | 17       | 0.13          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD13 | 17       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 20       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 20       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 20       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 20       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 20       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 20       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 26       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 26       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 26       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 26       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 26       | 0.13          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 26       | 0.13          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 31       | 0.13          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 31       | 0.13          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 31       | 0.13          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 31       | 0.13          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 31       | 0.13          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 31       | 0.13          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 21       | 0.13          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 28       | 0.13          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 28       | 0.13          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 28       | 0.13          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 33       | 0.13          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 33       | 0.13          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 33       | 0.13          |
| (1,1067) | 1:49:A:LEU:HD11 | 1:54:A:LEU:H    | 9        | 0.13          |
| (1,1067) | 1:49:A:LEU:HD12 | 1:54:A:LEU:H    | 9        | 0.13          |
| (1,1067) | 1:49:A:LEU:HD13 | 1:54:A:LEU:H    | 9        | 0.13          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 34       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 37       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 37       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 37       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 45       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 45       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 45       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 46       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 46       | 0.13          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 46       | 0.13          |
| (1,942)  | 1:33:A:LEU:HG   | 1:34:A:GLU:H    | 38       | 0.13          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 22       | 0.13          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 22       | 0.13          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 22       | 0.13          |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 31       | 0.13          |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 37       | 0.13          |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE2  | 50       | 0.13          |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE3  | 50       | 0.13          |
| (1,773)  | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE1  | 34       | 0.13          |
| (1,773)  | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE2  | 34       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,773) | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE1  | 34       | 0.13          |
| (1,773) | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE2  | 34       | 0.13          |
| (1,773) | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE1  | 34       | 0.13          |
| (1,773) | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE2  | 34       | 0.13          |
| (1,663) | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 31       | 0.13          |
| (1,663) | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 31       | 0.13          |
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 31       | 0.13          |
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 31       | 0.13          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 31       | 0.13          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 31       | 0.13          |
| (1,567) | 1:58:A:ILE:HD11 | 1:59:A:ASN:H    | 47       | 0.13          |
| (1,567) | 1:58:A:ILE:HD12 | 1:59:A:ASN:H    | 47       | 0.13          |
| (1,567) | 1:58:A:ILE:HD13 | 1:59:A:ASN:H    | 47       | 0.13          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 5        | 0.13          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 5        | 0.13          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 5        | 0.13          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 38       | 0.13          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 38       | 0.13          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 38       | 0.13          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 17       | 0.13          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 17       | 0.13          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 17       | 0.13          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 47       | 0.13          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 47       | 0.13          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 47       | 0.13          |
| (1,491) | 1:51:A:GLU:H    | 1:52:A:THR:HG21 | 17       | 0.13          |
| (1,491) | 1:51:A:GLU:H    | 1:52:A:THR:HG22 | 17       | 0.13          |
| (1,491) | 1:51:A:GLU:H    | 1:52:A:THR:HG23 | 17       | 0.13          |
| (1,463) | 1:49:A:LEU:HD11 | 1:55:A:GLY:H    | 22       | 0.13          |
| (1,463) | 1:49:A:LEU:HD12 | 1:55:A:GLY:H    | 22       | 0.13          |
| (1,463) | 1:49:A:LEU:HD13 | 1:55:A:GLY:H    | 22       | 0.13          |
| (1,463) | 1:49:A:LEU:HD11 | 1:55:A:GLY:H    | 43       | 0.13          |
| (1,463) | 1:49:A:LEU:HD12 | 1:55:A:GLY:H    | 43       | 0.13          |
| (1,463) | 1:49:A:LEU:HD13 | 1:55:A:GLY:H    | 43       | 0.13          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD11 | 5        | 0.13          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD12 | 5        | 0.13          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD13 | 5        | 0.13          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD11 | 5        | 0.13          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD12 | 5        | 0.13          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD13 | 5        | 0.13          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD11 | 5        | 0.13          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD12 | 5        | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD13 | 5        | 0.13          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD11 | 25       | 0.13          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD12 | 25       | 0.13          |
| (1,456) | 1:49:A:LEU:HD11 | 1:85:A:ILE:HD13 | 25       | 0.13          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD11 | 25       | 0.13          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD12 | 25       | 0.13          |
| (1,456) | 1:49:A:LEU:HD12 | 1:85:A:ILE:HD13 | 25       | 0.13          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD11 | 25       | 0.13          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD12 | 25       | 0.13          |
| (1,456) | 1:49:A:LEU:HD13 | 1:85:A:ILE:HD13 | 25       | 0.13          |
| (1,451) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 36       | 0.13          |
| (1,451) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 36       | 0.13          |
| (1,451) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 36       | 0.13          |
| (1,451) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 46       | 0.13          |
| (1,451) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 46       | 0.13          |
| (1,451) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 46       | 0.13          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 25       | 0.13          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 27       | 0.13          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 27       | 0.13          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 27       | 0.13          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 27       | 0.13          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 27       | 0.13          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 27       | 0.13          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 27       | 0.13          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 27       | 0.13          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 27       | 0.13          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 20       | 0.13          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 20       | 0.13          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 20       | 0.13          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 20       | 0.13          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 20       | 0.13          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 20       | 0.13          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 20       | 0.13          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 20       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 20       | 0.13          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 39       | 0.13          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 39       | 0.13          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 39       | 0.13          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 39       | 0.13          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 39       | 0.13          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 39       | 0.13          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 39       | 0.13          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 39       | 0.13          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 39       | 0.13          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 5        | 0.13          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 5        | 0.13          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 5        | 0.13          |
| (1,414) | 1:44:A:ILE:HG21 | 1:52:A:THR:HB   | 12       | 0.13          |
| (1,414) | 1:44:A:ILE:HG22 | 1:52:A:THR:HB   | 12       | 0.13          |
| (1,414) | 1:44:A:ILE:HG23 | 1:52:A:THR:HB   | 12       | 0.13          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 22       | 0.13          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 22       | 0.13          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 22       | 0.13          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 30       | 0.13          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 30       | 0.13          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 30       | 0.13          |
| (1,410) | 1:44:A:ILE:HG21 | 1:49:A:LEU:HG   | 50       | 0.13          |
| (1,410) | 1:44:A:ILE:HG22 | 1:49:A:LEU:HG   | 50       | 0.13          |
| (1,410) | 1:44:A:ILE:HG23 | 1:49:A:LEU:HG   | 50       | 0.13          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 45       | 0.13          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 45       | 0.13          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 45       | 0.13          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 46       | 0.13          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 46       | 0.13          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 46       | 0.13          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 5        | 0.13          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 5        | 0.13          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 5        | 0.13          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 5        | 0.13          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 5        | 0.13          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 5        | 0.13          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 5        | 0.13          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 5        | 0.13          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 5        | 0.13          |
| (1,370) | 1:7:A:ALA:HB1   | 1:42:A:TYR:HE1  | 18       | 0.13          |
| (1,370) | 1:7:A:ALA:HB1   | 1:42:A:TYR:HE2  | 18       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,370) | 1:7:A:ALA:HB2   | 1:42:A:TYR:HE1  | 18       | 0.13          |
| (1,370) | 1:7:A:ALA:HB2   | 1:42:A:TYR:HE2  | 18       | 0.13          |
| (1,370) | 1:7:A:ALA:HB3   | 1:42:A:TYR:HE1  | 18       | 0.13          |
| (1,370) | 1:7:A:ALA:HB3   | 1:42:A:TYR:HE2  | 18       | 0.13          |
| (1,359) | 1:39:A:LEU:HA   | 1:42:A:TYR:HB3  | 40       | 0.13          |
| (1,259) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG21 | 49       | 0.13          |
| (1,259) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG22 | 49       | 0.13          |
| (1,259) | 1:29:A:MET:HE1  | 1:32:A:VAL:HG23 | 49       | 0.13          |
| (1,259) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG21 | 49       | 0.13          |
| (1,259) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG22 | 49       | 0.13          |
| (1,259) | 1:29:A:MET:HE2  | 1:32:A:VAL:HG23 | 49       | 0.13          |
| (1,259) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG21 | 49       | 0.13          |
| (1,259) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG22 | 49       | 0.13          |
| (1,259) | 1:29:A:MET:HE3  | 1:32:A:VAL:HG23 | 49       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 15       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 20       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 48       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 48       | 0.13          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 48       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 48       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 48       | 0.13          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 48       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 48       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 48       | 0.13          |
| (1,224) | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 48       | 0.13          |
| (1,40)  | 1:12:A:ILE:HD11 | 1:39:A:LEU:HG   | 20       | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,40)   | 1:12:A:ILE:HD12 | 1:39:A:LEU:HG   | 20       | 0.13          |
| (1,40)   | 1:12:A:ILE:HD13 | 1:39:A:LEU:HG   | 20       | 0.13          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 26       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 26       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 26       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 26       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 26       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 26       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 37       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 37       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 37       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 37       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 37       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 37       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 39       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 39       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 39       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 39       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 39       | 0.12          |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 39       | 0.12          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 3        | 0.12          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 3        | 0.12          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 3        | 0.12          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 3        | 0.12          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 3        | 0.12          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 3        | 0.12          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB2  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD11 | 1:73:A:ARG:HB3  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB2  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD12 | 1:73:A:ARG:HB3  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB2  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD13 | 1:73:A:ARG:HB3  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB2  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD21 | 1:73:A:ARG:HB3  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB2  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD22 | 1:73:A:ARG:HB3  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB2  | 17       | 0.12          |
| (1,1748) | 1:70:A:LEU:HD23 | 1:73:A:ARG:HB3  | 17       | 0.12          |
| (1,1737) | 1:68:A:GLU:HG2  | 1:69:A:GLU:H    | 8        | 0.12          |
| (1,1737) | 1:68:A:GLU:HG3  | 1:69:A:GLU:H    | 8        | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 21       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 21       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 21       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 21       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 21       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 21       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 31       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 31       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 31       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 31       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 31       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 31       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 36       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 36       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 36       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 36       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 36       | 0.12          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 36       | 0.12          |
| (1,1576) | 1:46:A:LYS:HB2  | 1:85:A:ILE:HG21 | 7        | 0.12          |
| (1,1576) | 1:46:A:LYS:HB2  | 1:85:A:ILE:HG22 | 7        | 0.12          |
| (1,1576) | 1:46:A:LYS:HB2  | 1:85:A:ILE:HG23 | 7        | 0.12          |
| (1,1576) | 1:46:A:LYS:HB3  | 1:85:A:ILE:HG21 | 7        | 0.12          |
| (1,1576) | 1:46:A:LYS:HB3  | 1:85:A:ILE:HG22 | 7        | 0.12          |
| (1,1576) | 1:46:A:LYS:HB3  | 1:85:A:ILE:HG23 | 7        | 0.12          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD11 | 3        | 0.12          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD12 | 3        | 0.12          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD13 | 3        | 0.12          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD21 | 3        | 0.12          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD22 | 3        | 0.12          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD23 | 3        | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 18       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 18       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 18       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 18       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 18       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 18       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 19       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 19       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 19       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 19       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 19       | 0.12          |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 19       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 3        | 0.12          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 3        | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 3        | 0.12          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 3        | 0.12          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 3        | 0.12          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 3        | 0.12          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 31       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 31       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 31       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 31       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 31       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 31       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 36       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 36       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 36       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 36       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 36       | 0.12          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 36       | 0.12          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD11 | 49       | 0.12          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD12 | 49       | 0.12          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD13 | 49       | 0.12          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD21 | 49       | 0.12          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD22 | 49       | 0.12          |
| (1,1451) | 1:32:A:VAL:HB   | 1:33:A:LEU:HD23 | 49       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 15       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 15       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 15       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 15       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 34       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 34       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 34       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 34       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 40       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 40       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 40       | 0.12          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 40       | 0.12          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD11 | 36       | 0.12          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD12 | 36       | 0.12          |
| (1,1387) | 1:20:A:ILE:HG12 | 1:26:A:ILE:HD13 | 36       | 0.12          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD11 | 36       | 0.12          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD12 | 36       | 0.12          |
| (1,1387) | 1:20:A:ILE:HG13 | 1:26:A:ILE:HD13 | 36       | 0.12          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H    | 36       | 0.12          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H    | 36       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H    | 36       | 0.12          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H    | 36       | 0.12          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H    | 36       | 0.12          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H    | 36       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 33       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 33       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 33       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 33       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 33       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 33       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H    | 45       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H    | 45       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H    | 45       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H    | 45       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H    | 45       | 0.12          |
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 45       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD11 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD12 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD13 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD21 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD22 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD2  | 1:57:A:LEU:HD23 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD11 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD12 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD13 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD21 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD22 | 46       | 0.12          |
| (1,1309) | 1:13:A:ARG:HD3  | 1:57:A:LEU:HD23 | 46       | 0.12          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 18       | 0.12          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 27       | 0.12          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 46       | 0.12          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 46       | 0.12          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 46       | 0.12          |
| (1,1067) | 1:49:A:LEU:HD11 | 1:54:A:LEU:H    | 8        | 0.12          |
| (1,1067) | 1:49:A:LEU:HD12 | 1:54:A:LEU:H    | 8        | 0.12          |
| (1,1067) | 1:49:A:LEU:HD13 | 1:54:A:LEU:H    | 8        | 0.12          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 36       | 0.12          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 49       | 0.12          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 49       | 0.12          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 49       | 0.12          |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 33       | 0.12          |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 36       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,873) | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 42       | 0.12          |
| (1,873) | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 50       | 0.12          |
| (1,773) | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE1  | 48       | 0.12          |
| (1,773) | 1:5:A:ALA:HB1   | 1:42:A:TYR:HE2  | 48       | 0.12          |
| (1,773) | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE1  | 48       | 0.12          |
| (1,773) | 1:5:A:ALA:HB2   | 1:42:A:TYR:HE2  | 48       | 0.12          |
| (1,773) | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE1  | 48       | 0.12          |
| (1,773) | 1:5:A:ALA:HB3   | 1:42:A:TYR:HE2  | 48       | 0.12          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD11 | 23       | 0.12          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD12 | 23       | 0.12          |
| (1,749) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD13 | 23       | 0.12          |
| (1,749) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD11 | 23       | 0.12          |
| (1,749) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD12 | 23       | 0.12          |
| (1,749) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD13 | 23       | 0.12          |
| (1,749) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD11 | 23       | 0.12          |
| (1,749) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD12 | 23       | 0.12          |
| (1,749) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD13 | 23       | 0.12          |
| (1,740) | 1:81:A:TRP:HD1  | 1:84:A:LEU:HG   | 25       | 0.12          |
| (1,663) | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE2  | 3        | 0.12          |
| (1,663) | 1:71:A:ALA:HB1  | 1:72:A:LYS:HE3  | 3        | 0.12          |
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE2  | 3        | 0.12          |
| (1,663) | 1:71:A:ALA:HB2  | 1:72:A:LYS:HE3  | 3        | 0.12          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE2  | 3        | 0.12          |
| (1,663) | 1:71:A:ALA:HB3  | 1:72:A:LYS:HE3  | 3        | 0.12          |
| (1,655) | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD21 | 38       | 0.12          |
| (1,655) | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD22 | 38       | 0.12          |
| (1,655) | 1:81:A:TRP:HD1  | 1:84:A:LEU:HD23 | 38       | 0.12          |
| (1,567) | 1:58:A:ILE:HD11 | 1:59:A:ASN:H    | 19       | 0.12          |
| (1,567) | 1:58:A:ILE:HD12 | 1:59:A:ASN:H    | 19       | 0.12          |
| (1,567) | 1:58:A:ILE:HD13 | 1:59:A:ASN:H    | 19       | 0.12          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 1        | 0.12          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 1        | 0.12          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 1        | 0.12          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 21       | 0.12          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 21       | 0.12          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 21       | 0.12          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 37       | 0.12          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 37       | 0.12          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 37       | 0.12          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 41       | 0.12          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 41       | 0.12          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 41       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 44       | 0.12          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 44       | 0.12          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 44       | 0.12          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 26       | 0.12          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 26       | 0.12          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 26       | 0.12          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 38       | 0.12          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 38       | 0.12          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 38       | 0.12          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD21 | 31       | 0.12          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD22 | 31       | 0.12          |
| (1,477) | 1:49:A:LEU:H    | 1:49:A:LEU:HD23 | 31       | 0.12          |
| (1,463) | 1:49:A:LEU:HD11 | 1:55:A:GLY:H    | 34       | 0.12          |
| (1,463) | 1:49:A:LEU:HD12 | 1:55:A:GLY:H    | 34       | 0.12          |
| (1,463) | 1:49:A:LEU:HD13 | 1:55:A:GLY:H    | 34       | 0.12          |
| (1,451) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 17       | 0.12          |
| (1,451) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 17       | 0.12          |
| (1,451) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 17       | 0.12          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 7        | 0.12          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 50       | 0.12          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 50       | 0.12          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 50       | 0.12          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 50       | 0.12          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 50       | 0.12          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 50       | 0.12          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 50       | 0.12          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 50       | 0.12          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 50       | 0.12          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 26       | 0.12          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 26       | 0.12          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 26       | 0.12          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 26       | 0.12          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 26       | 0.12          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 26       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 26       | 0.12          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 26       | 0.12          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 26       | 0.12          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 40       | 0.12          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 40       | 0.12          |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 40       | 0.12          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 40       | 0.12          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 40       | 0.12          |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 40       | 0.12          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 40       | 0.12          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 40       | 0.12          |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 40       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 10       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 15       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 21       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 47       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 47       | 0.12          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 47       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 47       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 47       | 0.12          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 47       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 47       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 47       | 0.12          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 47       | 0.12          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 28       | 0.12          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 28       | 0.12          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 28       | 0.12          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD11 | 8        | 0.12          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD12 | 8        | 0.12          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD13 | 8        | 0.12          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD11 | 35       | 0.12          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD12 | 35       | 0.12          |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD13 | 35       | 0.12          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 2        | 0.12          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 2        | 0.12          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 2        | 0.12          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 12       | 0.12          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 12       | 0.12          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 12       | 0.12          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 1        | 0.12          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 1        | 0.12          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 1        | 0.12          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 1        | 0.12          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 1        | 0.12          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 1        | 0.12          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 1        | 0.12          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 1        | 0.12          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 1        | 0.12          |
| (1,360) | 1:38:A:SER:H    | 1:42:A:TYR:HD1  | 30       | 0.12          |
| (1,360) | 1:38:A:SER:H    | 1:42:A:TYR:HD2  | 30       | 0.12          |
| (1,359) | 1:39:A:LEU:HA   | 1:42:A:TYR:HB3  | 32       | 0.12          |
| (1,227) | 1:26:A:ILE:HA   | 1:29:A:MET:HE1  | 33       | 0.12          |
| (1,227) | 1:26:A:ILE:HA   | 1:29:A:MET:HE2  | 33       | 0.12          |
| (1,227) | 1:26:A:ILE:HA   | 1:29:A:MET:HE3  | 33       | 0.12          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD21 | 38       | 0.12          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD22 | 38       | 0.12          |
| (1,224) | 1:29:A:MET:HE1  | 1:70:A:LEU:HD23 | 38       | 0.12          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD21 | 38       | 0.12          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD22 | 38       | 0.12          |
| (1,224) | 1:29:A:MET:HE2  | 1:70:A:LEU:HD23 | 38       | 0.12          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD21 | 38       | 0.12          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD22 | 38       | 0.12          |
| (1,224)  | 1:29:A:MET:HE3  | 1:70:A:LEU:HD23 | 38       | 0.12          |
| (1,154)  | 1:20:A:ILE:HG21 | 1:29:A:MET:HA   | 39       | 0.12          |
| (1,154)  | 1:20:A:ILE:HG22 | 1:29:A:MET:HA   | 39       | 0.12          |
| (1,154)  | 1:20:A:ILE:HG23 | 1:29:A:MET:HA   | 39       | 0.12          |
| (1,40)   | 1:12:A:ILE:HD11 | 1:39:A:LEU:HG   | 42       | 0.12          |
| (1,40)   | 1:12:A:ILE:HD12 | 1:39:A:LEU:HG   | 42       | 0.12          |
| (1,40)   | 1:12:A:ILE:HD13 | 1:39:A:LEU:HG   | 42       | 0.12          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 4        | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 4        | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 4        | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 4        | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 4        | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 4        | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 38       | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 38       | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 38       | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 38       | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 38       | 0.11          |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 38       | 0.11          |
| (1,1737) | 1:68:A:GLU:HG2  | 1:69:A:GLU:H    | 7        | 0.11          |
| (1,1737) | 1:68:A:GLU:HG3  | 1:69:A:GLU:H    | 7        | 0.11          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG11 | 26       | 0.11          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG12 | 26       | 0.11          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG13 | 26       | 0.11          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG21 | 26       | 0.11          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG22 | 26       | 0.11          |
| (1,1657) | 1:57:A:LEU:HA   | 1:61:A:VAL:HG23 | 26       | 0.11          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 26       | 0.11          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 26       | 0.11          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 26       | 0.11          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 26       | 0.11          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 26       | 0.11          |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 26       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 14       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 14       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD11 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD12 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD13 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD11 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD12 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD13 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD11 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD12 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD13 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 49       | 0.11          |
| (1,1582) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 49       | 0.11          |
| (1,1562) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HB2  | 3        | 0.11          |
| (1,1562) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HB3  | 3        | 0.11          |
| (1,1562) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HB2  | 3        | 0.11          |
| (1,1562) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HB3  | 3        | 0.11          |
| (1,1562) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HB2  | 3        | 0.11          |
| (1,1562) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HB3  | 3        | 0.11          |
| (1,1562) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HB2  | 38       | 0.11          |
| (1,1562) | 1:44:A:ILE:HG21 | 1:84:A:LEU:HB3  | 38       | 0.11          |
| (1,1562) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HB2  | 38       | 0.11          |
| (1,1562) | 1:44:A:ILE:HG22 | 1:84:A:LEU:HB3  | 38       | 0.11          |
| (1,1562) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HB2  | 38       | 0.11          |
| (1,1562) | 1:44:A:ILE:HG23 | 1:84:A:LEU:HB3  | 38       | 0.11          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD11 | 10       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD12 | 10       | 0.11          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD13 | 10       | 0.11          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD21 | 10       | 0.11          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD22 | 10       | 0.11          |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD23 | 10       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 32       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 32       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 32       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 32       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 32       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 32       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 40       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 40       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 40       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 40       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 40       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 40       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG12 | 42       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG21 | 1:58:A:ILE:HG13 | 42       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG12 | 42       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG22 | 1:58:A:ILE:HG13 | 42       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG12 | 42       | 0.11          |
| (1,1498) | 1:36:A:ILE:HG23 | 1:58:A:ILE:HG13 | 42       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 20       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 20       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 20       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 20       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 21       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 21       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 21       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 21       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 26       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 26       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 26       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 26       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 31       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 31       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 31       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 31       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 33       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 33       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 33       | 0.11          |

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| Key      | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3 | 33       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2 | 38       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3 | 38       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2 | 38       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3 | 38       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2 | 45       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3 | 45       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2 | 45       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3 | 45       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2 | 49       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3 | 49       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2 | 49       | 0.11          |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3 | 49       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H   | 5        | 0.11          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H   | 5        | 0.11          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H   | 5        | 0.11          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H   | 5        | 0.11          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H   | 5        | 0.11          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H   | 5        | 0.11          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H   | 14       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H   | 14       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H   | 14       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H   | 14       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H   | 14       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H   | 14       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H   | 30       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H   | 30       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H   | 30       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H   | 30       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H   | 30       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H   | 30       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD11 | 1:33:A:LEU:H   | 35       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD12 | 1:33:A:LEU:H   | 35       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD13 | 1:33:A:LEU:H   | 35       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD21 | 1:33:A:LEU:H   | 35       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD22 | 1:33:A:LEU:H   | 35       | 0.11          |
| (1,1345) | 1:16:A:LEU:HD23 | 1:33:A:LEU:H   | 35       | 0.11          |
| (1,1340) | 1:16:A:LEU:HD11 | 1:20:A:ILE:H   | 37       | 0.11          |
| (1,1340) | 1:16:A:LEU:HD12 | 1:20:A:ILE:H   | 37       | 0.11          |
| (1,1340) | 1:16:A:LEU:HD13 | 1:20:A:ILE:H   | 37       | 0.11          |
| (1,1340) | 1:16:A:LEU:HD21 | 1:20:A:ILE:H   | 37       | 0.11          |
| (1,1340) | 1:16:A:LEU:HD22 | 1:20:A:ILE:H   | 37       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1340) | 1:16:A:LEU:HD23 | 1:20:A:ILE:H    | 37       | 0.11          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 1        | 0.11          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 24       | 0.11          |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 37       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 29       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 29       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 29       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 37       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 37       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 37       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 38       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 38       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 38       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG21 | 43       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG22 | 43       | 0.11          |
| (1,1111) | 1:62:A:ARG:H    | 1:65:A:THR:HG23 | 43       | 0.11          |
| (1,1069) | 1:55:A:GLY:H    | 1:56:A:LYS:HB2  | 41       | 0.11          |
| (1,1069) | 1:55:A:GLY:H    | 1:56:A:LYS:HB3  | 41       | 0.11          |
| (1,1016) | 1:46:A:LYS:H    | 1:84:A:LEU:HG   | 5        | 0.11          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 32       | 0.11          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 32       | 0.11          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 32       | 0.11          |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 48       | 0.11          |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 48       | 0.11          |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 48       | 0.11          |
| (1,973)  | 1:39:A:LEU:H    | 1:39:A:LEU:HG   | 44       | 0.11          |
| (1,934)  | 1:29:A:MET:HE1  | 1:33:A:LEU:H    | 11       | 0.11          |
| (1,934)  | 1:29:A:MET:HE2  | 1:33:A:LEU:H    | 11       | 0.11          |
| (1,934)  | 1:29:A:MET:HE3  | 1:33:A:LEU:H    | 11       | 0.11          |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 38       | 0.11          |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 48       | 0.11          |
| (1,873)  | 1:16:A:LEU:HA   | 1:20:A:ILE:H    | 49       | 0.11          |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD11 | 8        | 0.11          |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD12 | 8        | 0.11          |
| (1,750)  | 1:46:A:LYS:HA   | 1:84:A:LEU:HD13 | 8        | 0.11          |
| (1,639)  | 1:66:A:LYS:HA   | 1:66:A:LYS:HD2  | 50       | 0.11          |
| (1,639)  | 1:66:A:LYS:HA   | 1:66:A:LYS:HD3  | 50       | 0.11          |
| (1,567)  | 1:58:A:ILE:HD11 | 1:59:A:ASN:H    | 32       | 0.11          |
| (1,567)  | 1:58:A:ILE:HD12 | 1:59:A:ASN:H    | 32       | 0.11          |
| (1,567)  | 1:58:A:ILE:HD13 | 1:59:A:ASN:H    | 32       | 0.11          |
| (1,565)  | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 6        | 0.11          |
| (1,565)  | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 6        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 6        | 0.11          |
| (1,565) | 1:58:A:ILE:HD11 | 1:81:A:TRP:HE3  | 7        | 0.11          |
| (1,565) | 1:58:A:ILE:HD12 | 1:81:A:TRP:HE3  | 7        | 0.11          |
| (1,565) | 1:58:A:ILE:HD13 | 1:81:A:TRP:HE3  | 7        | 0.11          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 19       | 0.11          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 19       | 0.11          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 19       | 0.11          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 43       | 0.11          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 43       | 0.11          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 43       | 0.11          |
| (1,542) | 1:57:A:LEU:HD21 | 1:58:A:ILE:H    | 50       | 0.11          |
| (1,542) | 1:57:A:LEU:HD22 | 1:58:A:ILE:H    | 50       | 0.11          |
| (1,542) | 1:57:A:LEU:HD23 | 1:58:A:ILE:H    | 50       | 0.11          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD21 | 41       | 0.11          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD22 | 41       | 0.11          |
| (1,528) | 1:13:A:ARG:H    | 1:54:A:LEU:HD23 | 41       | 0.11          |
| (1,484) | 1:48:A:ALA:HA   | 1:52:A:THR:HG21 | 49       | 0.11          |
| (1,484) | 1:48:A:ALA:HA   | 1:52:A:THR:HG22 | 49       | 0.11          |
| (1,484) | 1:48:A:ALA:HA   | 1:52:A:THR:HG23 | 49       | 0.11          |
| (1,463) | 1:49:A:LEU:HD11 | 1:55:A:GLY:H    | 8        | 0.11          |
| (1,463) | 1:49:A:LEU:HD12 | 1:55:A:GLY:H    | 8        | 0.11          |
| (1,463) | 1:49:A:LEU:HD13 | 1:55:A:GLY:H    | 8        | 0.11          |
| (1,455) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD21 | 33       | 0.11          |
| (1,455) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD22 | 33       | 0.11          |
| (1,455) | 1:49:A:LEU:HD11 | 1:84:A:LEU:HD23 | 33       | 0.11          |
| (1,455) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD21 | 33       | 0.11          |
| (1,455) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD22 | 33       | 0.11          |
| (1,455) | 1:49:A:LEU:HD12 | 1:84:A:LEU:HD23 | 33       | 0.11          |
| (1,455) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD21 | 33       | 0.11          |
| (1,455) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD22 | 33       | 0.11          |
| (1,455) | 1:49:A:LEU:HD13 | 1:84:A:LEU:HD23 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 1        | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 17       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 17       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 17       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 17       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 17       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 17       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 17       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 17       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 17       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 18       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 33       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD21 | 41       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD22 | 41       | 0.11          |
| (1,438) | 1:48:A:ALA:HB1  | 1:49:A:LEU:HD23 | 41       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD21 | 41       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD22 | 41       | 0.11          |
| (1,438) | 1:48:A:ALA:HB2  | 1:49:A:LEU:HD23 | 41       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD21 | 41       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD22 | 41       | 0.11          |
| (1,438) | 1:48:A:ALA:HB3  | 1:49:A:LEU:HD23 | 41       | 0.11          |
| (1,428) | 1:45:A:THR:HG21 | 1:47:A:GLU:H    | 46       | 0.11          |
| (1,428) | 1:45:A:THR:HG22 | 1:47:A:GLU:H    | 46       | 0.11          |
| (1,428) | 1:45:A:THR:HG23 | 1:47:A:GLU:H    | 46       | 0.11          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 1        | 0.11          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 1        | 0.11          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 1        | 0.11          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 1        | 0.11          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 1        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 1        | 0.11          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 1        | 0.11          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 1        | 0.11          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 1        | 0.11          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG21 | 20       | 0.11          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG22 | 20       | 0.11          |
| (1,423) | 1:44:A:ILE:HG21 | 1:45:A:THR:HG23 | 20       | 0.11          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG21 | 20       | 0.11          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG22 | 20       | 0.11          |
| (1,423) | 1:44:A:ILE:HG22 | 1:45:A:THR:HG23 | 20       | 0.11          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG21 | 20       | 0.11          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG22 | 20       | 0.11          |
| (1,423) | 1:44:A:ILE:HG23 | 1:45:A:THR:HG23 | 20       | 0.11          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG21 | 29       | 0.11          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG22 | 29       | 0.11          |
| (1,413) | 1:9:A:PRO:HA    | 1:44:A:ILE:HG23 | 29       | 0.11          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 36       | 0.11          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 36       | 0.11          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 36       | 0.11          |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 50       | 0.11          |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 50       | 0.11          |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 50       | 0.11          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 6        | 0.11          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 27       | 0.11          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD21 | 40       | 0.11          |
| (1,387) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD22 | 40       | 0.11          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,387)  | 1:44:A:ILE:HD11 | 1:49:A:LEU:HD23 | 40       | 0.11          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD21 | 40       | 0.11          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD22 | 40       | 0.11          |
| (1,387)  | 1:44:A:ILE:HD12 | 1:49:A:LEU:HD23 | 40       | 0.11          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD21 | 40       | 0.11          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD22 | 40       | 0.11          |
| (1,387)  | 1:44:A:ILE:HD13 | 1:49:A:LEU:HD23 | 40       | 0.11          |
| (1,360)  | 1:38:A:SER:H    | 1:42:A:TYR:HD1  | 18       | 0.11          |
| (1,360)  | 1:38:A:SER:H    | 1:42:A:TYR:HD2  | 18       | 0.11          |
| (1,360)  | 1:38:A:SER:H    | 1:42:A:TYR:HD1  | 44       | 0.11          |
| (1,360)  | 1:38:A:SER:H    | 1:42:A:TYR:HD2  | 44       | 0.11          |
| (1,335)  | 1:36:A:ILE:HG21 | 1:77:A:LEU:H    | 26       | 0.11          |
| (1,335)  | 1:36:A:ILE:HG22 | 1:77:A:LEU:H    | 26       | 0.11          |
| (1,335)  | 1:36:A:ILE:HG23 | 1:77:A:LEU:H    | 26       | 0.11          |
| (1,327)  | 1:36:A:ILE:HG21 | 1:40:A:GLU:HG2  | 31       | 0.11          |
| (1,327)  | 1:36:A:ILE:HG22 | 1:40:A:GLU:HG2  | 31       | 0.11          |
| (1,327)  | 1:36:A:ILE:HG23 | 1:40:A:GLU:HG2  | 31       | 0.11          |
| (1,252)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG11 | 41       | 0.11          |
| (1,252)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG12 | 41       | 0.11          |
| (1,252)  | 1:32:A:VAL:H    | 1:32:A:VAL:HG13 | 41       | 0.11          |
| (1,192)  | 1:26:A:ILE:HD11 | 1:32:A:VAL:H    | 25       | 0.11          |
| (1,192)  | 1:26:A:ILE:HD12 | 1:32:A:VAL:H    | 25       | 0.11          |
| (1,192)  | 1:26:A:ILE:HD13 | 1:32:A:VAL:H    | 25       | 0.11          |
| (1,154)  | 1:20:A:ILE:HG21 | 1:29:A:MET:HA   | 18       | 0.11          |
| (1,154)  | 1:20:A:ILE:HG22 | 1:29:A:MET:HA   | 18       | 0.11          |
| (1,154)  | 1:20:A:ILE:HG23 | 1:29:A:MET:HA   | 18       | 0.11          |
| (1,48)   | 1:12:A:ILE:HG21 | 1:39:A:LEU:HG   | 45       | 0.11          |
| (1,48)   | 1:12:A:ILE:HG22 | 1:39:A:LEU:HG   | 45       | 0.11          |
| (1,48)   | 1:12:A:ILE:HG23 | 1:39:A:LEU:HG   | 45       | 0.11          |
| (1,40)   | 1:12:A:ILE:HD11 | 1:39:A:LEU:HG   | 32       | 0.11          |
| (1,40)   | 1:12:A:ILE:HD12 | 1:39:A:LEU:HG   | 32       | 0.11          |
| (1,40)   | 1:12:A:ILE:HD13 | 1:39:A:LEU:HG   | 32       | 0.11          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD11 | 28       | 0.11          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD12 | 28       | 0.11          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD13 | 28       | 0.11          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD11 | 30       | 0.11          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD12 | 30       | 0.11          |
| (1,23)   | 1:9:A:PRO:HG2   | 1:12:A:ILE:HD13 | 30       | 0.11          |
| (1,1790) | 1:77:A:LEU:HD11 | 1:78:A:LEU:H    | 16       | 0.1           |
| (1,1790) | 1:77:A:LEU:HD12 | 1:78:A:LEU:H    | 16       | 0.1           |
| (1,1790) | 1:77:A:LEU:HD13 | 1:78:A:LEU:H    | 16       | 0.1           |
| (1,1790) | 1:77:A:LEU:HD21 | 1:78:A:LEU:H    | 16       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1790) | 1:77:A:LEU:HD22 | 1:78:A:LEU:H    | 16       | 0.1           |
| (1,1790) | 1:77:A:LEU:HD23 | 1:78:A:LEU:H    | 16       | 0.1           |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD11 | 19       | 0.1           |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD12 | 19       | 0.1           |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD13 | 19       | 0.1           |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD21 | 19       | 0.1           |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD22 | 19       | 0.1           |
| (1,1763) | 1:73:A:ARG:HA   | 1:77:A:LEU:HD23 | 19       | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 3        | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 3        | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 3        | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 3        | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 3        | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 3        | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD11 | 46       | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD12 | 46       | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD13 | 46       | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD21 | 46       | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD22 | 46       | 0.1           |
| (1,1625) | 1:53:A:ARG:HA   | 1:54:A:LEU:HD23 | 46       | 0.1           |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 2        | 0.1           |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 2        | 0.1           |
| (1,1588) | 1:49:A:LEU:HB2  | 1:53:A:ARG:H    | 12       | 0.1           |
| (1,1588) | 1:49:A:LEU:HB3  | 1:53:A:ARG:H    | 12       | 0.1           |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD11 | 8        | 0.1           |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD12 | 8        | 0.1           |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD13 | 8        | 0.1           |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD21 | 8        | 0.1           |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD22 | 8        | 0.1           |
| (1,1557) | 1:44:A:ILE:HB   | 1:49:A:LEU:HD23 | 8        | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 8        | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 8        | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 8        | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 8        | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 8        | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 8        | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 37       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 37       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 37       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 37       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 37       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 37       | 0.1           |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD11 | 42       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD12 | 42       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD13 | 42       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD21 | 42       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD22 | 42       | 0.1           |
| (1,1555) | 1:44:A:ILE:H    | 1:54:A:LEU:HD23 | 42       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 4        | 0.1           |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 4        | 0.1           |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 4        | 0.1           |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 4        | 0.1           |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 14       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 14       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 14       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 14       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 36       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 36       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 36       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 36       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD2  | 41       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB2  | 1:22:A:PRO:HD3  | 41       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD2  | 41       | 0.1           |
| (1,1394) | 1:21:A:ASP:HB3  | 1:22:A:PRO:HD3  | 41       | 0.1           |
| (1,1242) | 1:84:A:LEU:H    | 1:84:A:LEU:HG   | 40       | 0.1           |
| (1,1233) | 1:82:A:GLN:H    | 1:82:A:GLN:HG2  | 38       | 0.1           |
| (1,993)  | 1:36:A:ILE:HD11 | 1:40:A:GLU:H    | 18       | 0.1           |
| (1,993)  | 1:36:A:ILE:HD12 | 1:40:A:GLU:H    | 18       | 0.1           |
| (1,993)  | 1:36:A:ILE:HD13 | 1:40:A:GLU:H    | 18       | 0.1           |
| (1,838)  | 1:15:A:ARG:H    | 1:35:A:VAL:HG11 | 45       | 0.1           |
| (1,838)  | 1:15:A:ARG:H    | 1:35:A:VAL:HG12 | 45       | 0.1           |
| (1,838)  | 1:15:A:ARG:H    | 1:35:A:VAL:HG13 | 45       | 0.1           |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE2  | 33       | 0.1           |
| (1,775)  | 1:64:A:LYS:H    | 1:64:A:LYS:HE3  | 33       | 0.1           |
| (1,764)  | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG21 | 33       | 0.1           |
| (1,764)  | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG22 | 33       | 0.1           |
| (1,764)  | 1:46:A:LYS:HE2  | 1:85:A:ILE:HG23 | 33       | 0.1           |
| (1,764)  | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG21 | 33       | 0.1           |
| (1,764)  | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG22 | 33       | 0.1           |
| (1,764)  | 1:46:A:LYS:HE3  | 1:85:A:ILE:HG23 | 33       | 0.1           |
| (1,701)  | 1:74:A:ALA:HA   | 1:77:A:LEU:HB3  | 26       | 0.1           |
| (1,674)  | 1:73:A:ARG:H    | 1:73:A:ARG:HD3  | 21       | 0.1           |
| (1,630)  | 1:63:A:LYS:HA   | 1:65:A:THR:HG21 | 34       | 0.1           |
| (1,630)  | 1:63:A:LYS:HA   | 1:65:A:THR:HG22 | 34       | 0.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,630) | 1:63:A:LYS:HA   | 1:65:A:THR:HG23 | 34       | 0.1           |
| (1,567) | 1:58:A:ILE:HD11 | 1:59:A:ASN:H    | 37       | 0.1           |
| (1,567) | 1:58:A:ILE:HD12 | 1:59:A:ASN:H    | 37       | 0.1           |
| (1,567) | 1:58:A:ILE:HD13 | 1:59:A:ASN:H    | 37       | 0.1           |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD2  | 18       | 0.1           |
| (1,495) | 1:53:A:ARG:HA   | 1:53:A:ARG:HD3  | 18       | 0.1           |
| (1,469) | 1:49:A:LEU:HD21 | 1:54:A:LEU:HB2  | 36       | 0.1           |
| (1,469) | 1:49:A:LEU:HD22 | 1:54:A:LEU:HB2  | 36       | 0.1           |
| (1,469) | 1:49:A:LEU:HD23 | 1:54:A:LEU:HB2  | 36       | 0.1           |
| (1,463) | 1:49:A:LEU:HD11 | 1:55:A:GLY:H    | 13       | 0.1           |
| (1,463) | 1:49:A:LEU:HD12 | 1:55:A:GLY:H    | 13       | 0.1           |
| (1,463) | 1:49:A:LEU:HD13 | 1:55:A:GLY:H    | 13       | 0.1           |
| (1,454) | 1:49:A:LEU:HG   | 1:55:A:GLY:HA3  | 26       | 0.1           |
| (1,454) | 1:49:A:LEU:HG   | 1:55:A:GLY:HA3  | 28       | 0.1           |
| (1,454) | 1:49:A:LEU:HG   | 1:55:A:GLY:HA3  | 34       | 0.1           |
| (1,451) | 1:44:A:ILE:HD11 | 1:49:A:LEU:HG   | 15       | 0.1           |
| (1,451) | 1:44:A:ILE:HD12 | 1:49:A:LEU:HG   | 15       | 0.1           |
| (1,451) | 1:44:A:ILE:HD13 | 1:49:A:LEU:HG   | 15       | 0.1           |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB1  | 18       | 0.1           |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB2  | 18       | 0.1           |
| (1,435) | 1:44:A:ILE:HG21 | 1:48:A:ALA:HB3  | 18       | 0.1           |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB1  | 18       | 0.1           |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB2  | 18       | 0.1           |
| (1,435) | 1:44:A:ILE:HG22 | 1:48:A:ALA:HB3  | 18       | 0.1           |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB1  | 18       | 0.1           |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB2  | 18       | 0.1           |
| (1,435) | 1:44:A:ILE:HG23 | 1:48:A:ALA:HB3  | 18       | 0.1           |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD11 | 19       | 0.1           |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD12 | 19       | 0.1           |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD13 | 19       | 0.1           |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD11 | 20       | 0.1           |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD12 | 20       | 0.1           |
| (1,404) | 1:44:A:ILE:H    | 1:44:A:ILE:HD13 | 20       | 0.1           |
| (1,402) | 1:44:A:ILE:HD11 | 1:45:A:THR:H    | 13       | 0.1           |
| (1,402) | 1:44:A:ILE:HD12 | 1:45:A:THR:H    | 13       | 0.1           |
| (1,402) | 1:44:A:ILE:HD13 | 1:45:A:THR:H    | 13       | 0.1           |
| (1,360) | 1:38:A:SER:H    | 1:42:A:TYR:HD1  | 31       | 0.1           |
| (1,360) | 1:38:A:SER:H    | 1:42:A:TYR:HD2  | 31       | 0.1           |
| (1,240) | 1:28:A:ASN:HB2  | 1:31:A:ALA:HB1  | 37       | 0.1           |
| (1,240) | 1:28:A:ASN:HB2  | 1:31:A:ALA:HB2  | 37       | 0.1           |
| (1,240) | 1:28:A:ASN:HB2  | 1:31:A:ALA:HB3  | 37       | 0.1           |
| (1,227) | 1:26:A:ILE:HA   | 1:29:A:MET:HE1  | 40       | 0.1           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,227) | 1:26:A:ILE:HA  | 1:29:A:MET:HE2  | 40       | 0.1           |
| (1,227) | 1:26:A:ILE:HA  | 1:29:A:MET:HE3  | 40       | 0.1           |
| (1,224) | 1:29:A:MET:HE1 | 1:70:A:LEU:HD21 | 14       | 0.1           |
| (1,224) | 1:29:A:MET:HE1 | 1:70:A:LEU:HD22 | 14       | 0.1           |
| (1,224) | 1:29:A:MET:HE1 | 1:70:A:LEU:HD23 | 14       | 0.1           |
| (1,224) | 1:29:A:MET:HE2 | 1:70:A:LEU:HD21 | 14       | 0.1           |
| (1,224) | 1:29:A:MET:HE2 | 1:70:A:LEU:HD22 | 14       | 0.1           |
| (1,224) | 1:29:A:MET:HE2 | 1:70:A:LEU:HD23 | 14       | 0.1           |
| (1,224) | 1:29:A:MET:HE3 | 1:70:A:LEU:HD21 | 14       | 0.1           |
| (1,224) | 1:29:A:MET:HE3 | 1:70:A:LEU:HD22 | 14       | 0.1           |
| (1,224) | 1:29:A:MET:HE3 | 1:70:A:LEU:HD23 | 14       | 0.1           |
| (1,222) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG11 | 41       | 0.1           |
| (1,222) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG12 | 41       | 0.1           |
| (1,222) | 1:29:A:MET:HE1 | 1:32:A:VAL:HG13 | 41       | 0.1           |
| (1,222) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG11 | 41       | 0.1           |
| (1,222) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG12 | 41       | 0.1           |
| (1,222) | 1:29:A:MET:HE2 | 1:32:A:VAL:HG13 | 41       | 0.1           |
| (1,222) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG11 | 41       | 0.1           |
| (1,222) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG12 | 41       | 0.1           |
| (1,222) | 1:29:A:MET:HE3 | 1:32:A:VAL:HG13 | 41       | 0.1           |
| (1,23)  | 1:9:A:PRO:HG2  | 1:12:A:ILE:HD11 | 15       | 0.1           |
| (1,23)  | 1:9:A:PRO:HG2  | 1:12:A:ILE:HD12 | 15       | 0.1           |
| (1,23)  | 1:9:A:PRO:HG2  | 1:12:A:ILE:HD13 | 15       | 0.1           |

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

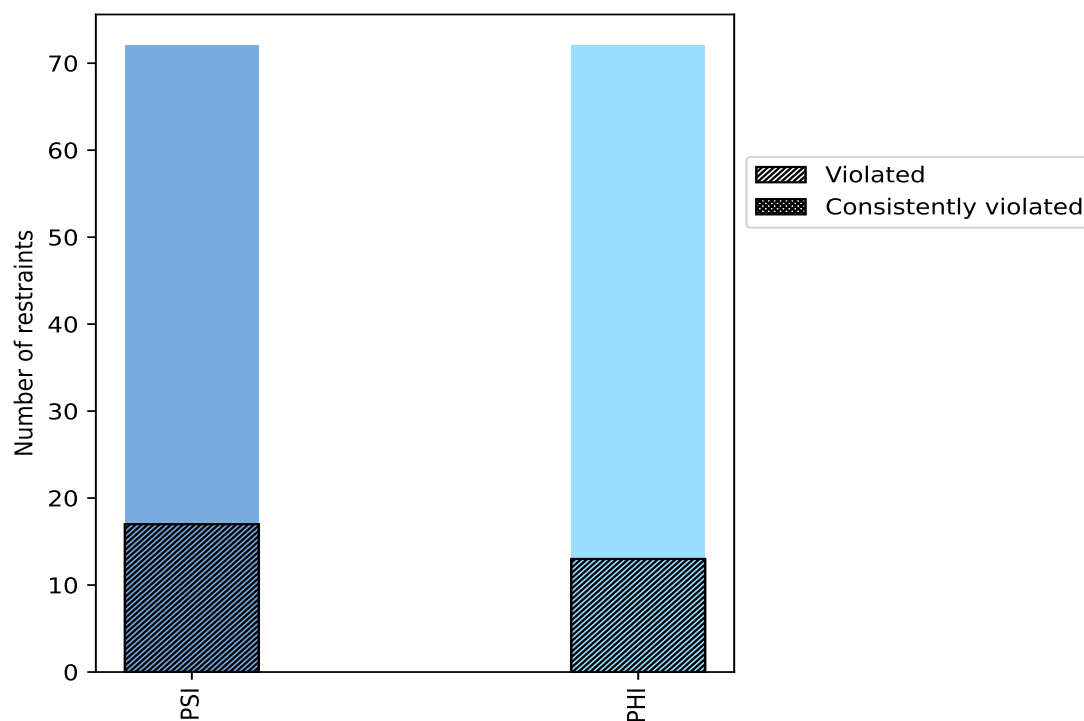
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| PSI        | 72    | 50.0           | 17                    | 23.6           | 11.8           | 0                                  | 0.0            | 0.0            |
| PHI        | 72    | 50.0           | 13                    | 18.1           | 9.0            | 0                                  | 0.0            | 0.0            |
| Total      | 144   | 100.0          | 30                    | 20.8           | 20.8           | 0                                  | 0.0            | 0.0            |

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

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



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

## 10.2 Dihedral-angle violation statistics for each model [i](#)

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 (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 0                    | 2   | 2     | 3.84     | 4.27    | 0.42   | 3.84       |
| 2        | 0                    | 1   | 1     | 4.91     | 4.91    | 0.0    | 4.91       |
| 3        | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 4        | 2                    | 2   | 4     | 2.89     | 3.81    | 0.8    | 2.92       |
| 5        | 1                    | 3   | 4     | 4.03     | 4.78    | 0.67   | 4.09       |
| 6        | 0                    | 1   | 1     | 4.92     | 4.92    | 0.0    | 4.92       |
| 7        | 0                    | 3   | 3     | 3.23     | 4.78    | 1.48   | 3.68       |
| 8        | 0                    | 2   | 2     | 3.02     | 3.1     | 0.08   | 3.02       |
| 9        | 3                    | 2   | 5     | 1.89     | 3.63    | 0.92   | 1.4        |
| 10       | 0                    | 1   | 1     | 4.92     | 4.92    | 0.0    | 4.92       |
| 11       | 0                    | 1   | 1     | 3.81     | 3.81    | 0.0    | 3.81       |
| 12       | 2                    | 3   | 5     | 2.83     | 3.85    | 0.78   | 2.78       |
| 13       | 1                    | 1   | 2     | 2.14     | 3.13    | 0.99   | 2.14       |
| 14       | 1                    | 1   | 2     | 3.31     | 4.5     | 1.19   | 3.31       |
| 15       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 16       | 0                    | 2   | 2     | 2.72     | 3.9     | 1.18   | 2.72       |
| 17       | 1                    | 1   | 2     | 3.61     | 3.85    | 0.24   | 3.61       |
| 18       | 1                    | 3   | 4     | 2.93     | 4.13    | 0.85   | 2.88       |
| 19       | 1                    | 3   | 4     | 2.51     | 3.33    | 0.76   | 2.7        |
| 20       | 1                    | 1   | 2     | 4.08     | 4.89    | 0.8    | 4.08       |
| 21       | 3                    | 2   | 5     | 2.04     | 3.29    | 0.84   | 1.96       |
| 22       | 2                    | 1   | 3     | 2.66     | 3.68    | 1.04   | 3.06       |
| 23       | 1                    | 2   | 3     | 3.42     | 4.66    | 1.13   | 3.69       |
| 24       | 1                    | 1   | 2     | 4.08     | 4.47    | 0.38   | 4.08       |
| 25       | 2                    | 3   | 5     | 2.15     | 2.66    | 0.48   | 2.29       |
| 26       | 1                    | 0   | 1     | 2.57     | 2.57    | 0.0    | 2.57       |
| 27       | 1                    | 1   | 2     | 3.26     | 3.48    | 0.22   | 3.26       |
| 28       | 4                    | 0   | 4     | 1.54     | 1.78    | 0.19   | 1.57       |
| 29       | 1                    | 0   | 1     | 1.58     | 1.58    | 0.0    | 1.58       |
| 30       | 1                    | 3   | 4     | 2.05     | 4.0     | 1.15   | 1.6        |
| 31       | 1                    | 1   | 2     | 1.66     | 1.7     | 0.04   | 1.66       |
| 32       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 33       | 1                    | 1   | 2     | 4.3      | 4.44    | 0.14   | 4.3        |
| 34       | 1                    | 1   | 2     | 1.48     | 1.68    | 0.2    | 1.48       |
| 35       | 1                    | 3   | 4     | 3.2      | 4.44    | 0.92   | 3.05       |
| 36       | 0                    | 1   | 1     | 1.4      | 1.4     | 0.0    | 1.4        |
| 37       | 0                    | 3   | 3     | 2.81     | 4.12    | 1.11   | 2.92       |
| 38       | 2                    | 0   | 2     | 3.72     | 4.07    | 0.35   | 3.72       |

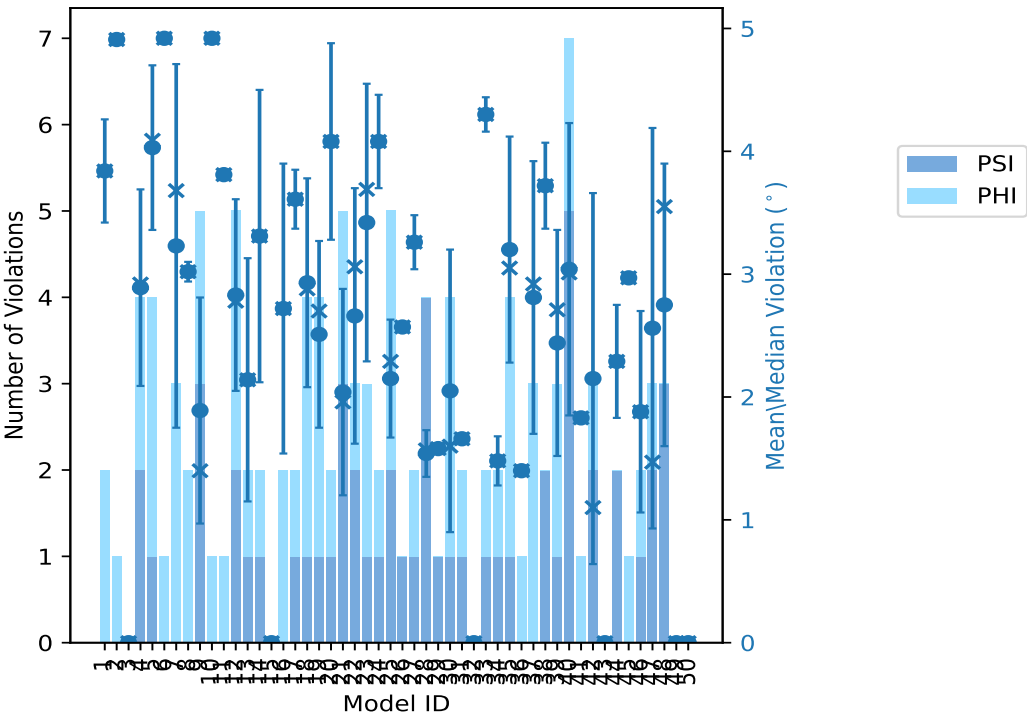
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| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 39       | 1                    | 2   | 3     | 2.44     | 3.41    | 0.92   | 2.71       |
| 40       | 5                    | 2   | 7     | 3.04     | 4.84    | 1.19   | 3.01       |
| 41       | 0                    | 1   | 1     | 1.83     | 1.83    | 0.0    | 1.83       |
| 42       | 2                    | 1   | 3     | 2.15     | 4.28    | 1.51   | 1.1        |
| 43       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 44       | 2                    | 0   | 2     | 2.29     | 2.75    | 0.46   | 2.29       |
| 45       | 0                    | 1   | 1     | 2.97     | 2.97    | 0.0    | 2.97       |
| 46       | 1                    | 1   | 2     | 1.88     | 2.69    | 0.82   | 1.88       |
| 47       | 2                    | 1   | 3     | 2.56     | 4.86    | 1.63   | 1.47       |
| 48       | 3                    | 0   | 3     | 2.75     | 3.57    | 1.15   | 3.55       |
| 49       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |
| 50       | 0                    | 0   | 0     | 0.0      | 0.0     | 0.0    | 0.0        |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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 |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 4                             | 4   | 8     | 1                        | 2.0  |
| 9                             | 3   | 12    | 2                        | 4.0  |
| 0                             | 2   | 2     | 3                        | 6.0  |
| 1                             | 0   | 1     | 4                        | 8.0  |
| 1                             | 1   | 2     | 5                        | 10.0 |
| 0                             | 0   | 0     | 6                        | 12.0 |
| 0                             | 1   | 1     | 7                        | 14.0 |
| 0                             | 0   | 0     | 8                        | 16.0 |
| 0                             | 0   | 0     | 9                        | 18.0 |
| 1                             | 0   | 1     | 10                       | 20.0 |
| 0                             | 0   | 0     | 11                       | 22.0 |
| 1                             | 0   | 1     | 12                       | 24.0 |
| 0                             | 0   | 0     | 13                       | 26.0 |
| 0                             | 0   | 0     | 14                       | 28.0 |
| 0                             | 0   | 0     | 15                       | 30.0 |
| 0                             | 1   | 1     | 16                       | 32.0 |
| 0                             | 0   | 0     | 17                       | 34.0 |
| 0                             | 0   | 0     | 18                       | 36.0 |
| 0                             | 0   | 0     | 19                       | 38.0 |
| 0                             | 0   | 0     | 20                       | 40.0 |
| 0                             | 1   | 1     | 21                       | 42.0 |
| 0                             | 0   | 0     | 22                       | 44.0 |
| 0                             | 0   | 0     | 23                       | 46.0 |
| 0                             | 0   | 0     | 24                       | 48.0 |
| 0                             | 0   | 0     | 25                       | 50.0 |
| 0                             | 0   | 0     | 26                       | 52.0 |
| 0                             | 0   | 0     | 27                       | 54.0 |
| 0                             | 0   | 0     | 28                       | 56.0 |
| 0                             | 0   | 0     | 29                       | 58.0 |
| 0                             | 0   | 0     | 30                       | 60.0 |
| 0                             | 0   | 0     | 31                       | 62.0 |
| 0                             | 0   | 0     | 32                       | 64.0 |
| 0                             | 0   | 0     | 33                       | 66.0 |
| 0                             | 0   | 0     | 34                       | 68.0 |
| 0                             | 0   | 0     | 35                       | 70.0 |
| 0                             | 0   | 0     | 36                       | 72.0 |
| 0                             | 0   | 0     | 37                       | 74.0 |

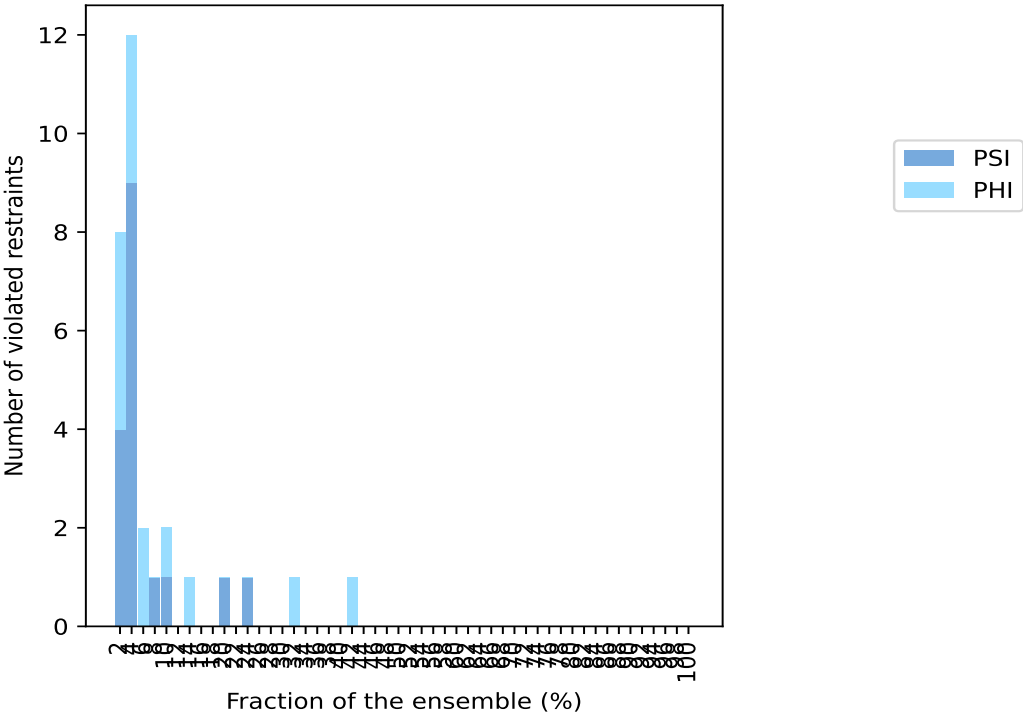
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 38                       | 76.0  |
| 0                             | 0   | 0     | 39                       | 78.0  |
| 0                             | 0   | 0     | 40                       | 80.0  |
| 0                             | 0   | 0     | 41                       | 82.0  |
| 0                             | 0   | 0     | 42                       | 84.0  |
| 0                             | 0   | 0     | 43                       | 86.0  |
| 0                             | 0   | 0     | 44                       | 88.0  |
| 0                             | 0   | 0     | 45                       | 90.0  |
| 0                             | 0   | 0     | 46                       | 92.0  |
| 0                             | 0   | 0     | 47                       | 94.0  |
| 0                             | 0   | 0     | 48                       | 96.0  |
| 0                             | 0   | 0     | 49                       | 98.0  |
| 0                             | 0   | 0     | 50                       | 100.0 |

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

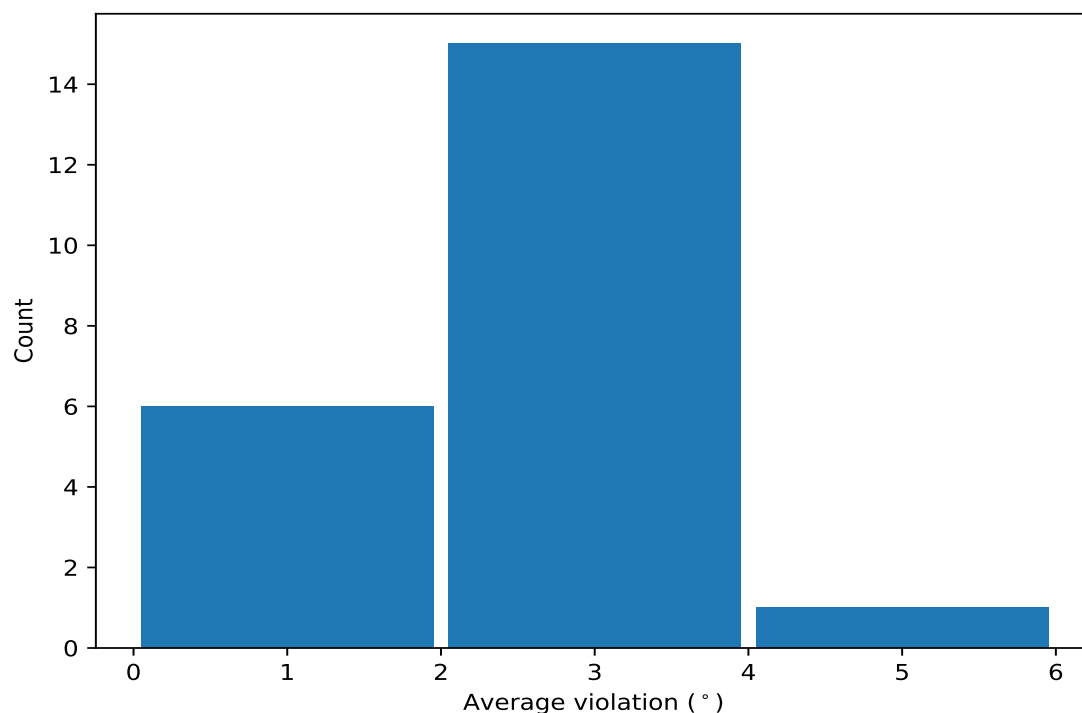
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



## 10.4 Most violated dihedral-angle restraints in the ensemble [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 |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 21                  | 3.06 | 1.3             | 3.13   |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 16                  | 3.74 | 0.64            | 3.66   |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 12                  | 2.75 | 1.01            | 2.88   |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 10                  | 2.59 | 1.15            | 2.82   |
| (1,87)  | 1:55:A:GLY:C | 1:56:A:LYS:N  | 1:56:A:LYS:CA | 1:56:A:LYS:C | 7                   | 3.0  | 0.93            | 2.65   |
| (1,7)   | 1:10:A:GLN:C | 1:11:A:GLN:N  | 1:11:A:GLN:CA | 1:11:A:GLN:C | 5                   | 2.11 | 0.52            | 1.75   |
| (1,144) | 1:85:A:ILE:N | 1:85:A:ILE:CA | 1:85:A:ILE:C  | 1:86:A:GLU:N | 5                   | 1.89 | 0.64            | 1.7    |
| (1,16)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:LEU:N | 4                   | 2.22 | 0.84            | 2.12   |
| (1,71)  | 1:47:A:GLU:C | 1:48:A:ALA:N  | 1:48:A:ALA:CA | 1:48:A:ALA:C | 3                   | 3.37 | 1.68            | 4.44   |
| (1,139) | 1:82:A:GLN:C | 1:83:A:LYS:N  | 1:83:A:LYS:CA | 1:83:A:LYS:C | 3                   | 2.43 | 0.92            | 1.83   |
| (1,66)  | 1:45:A:THR:N | 1:45:A:THR:CA | 1:45:A:THR:C  | 1:46:A:LYS:N | 2                   | 4.26 | 0.57            | 4.26   |
| (1,82)  | 1:53:A:ARG:N | 1:53:A:ARG:CA | 1:53:A:ARG:C  | 1:54:A:LEU:N | 2                   | 2.96 | 0.19            | 2.96   |
| (1,103) | 1:63:A:LYS:C | 1:64:A:LYS:N  | 1:64:A:LYS:CA | 1:64:A:LYS:C | 2                   | 2.85 | 0.48            | 2.85   |

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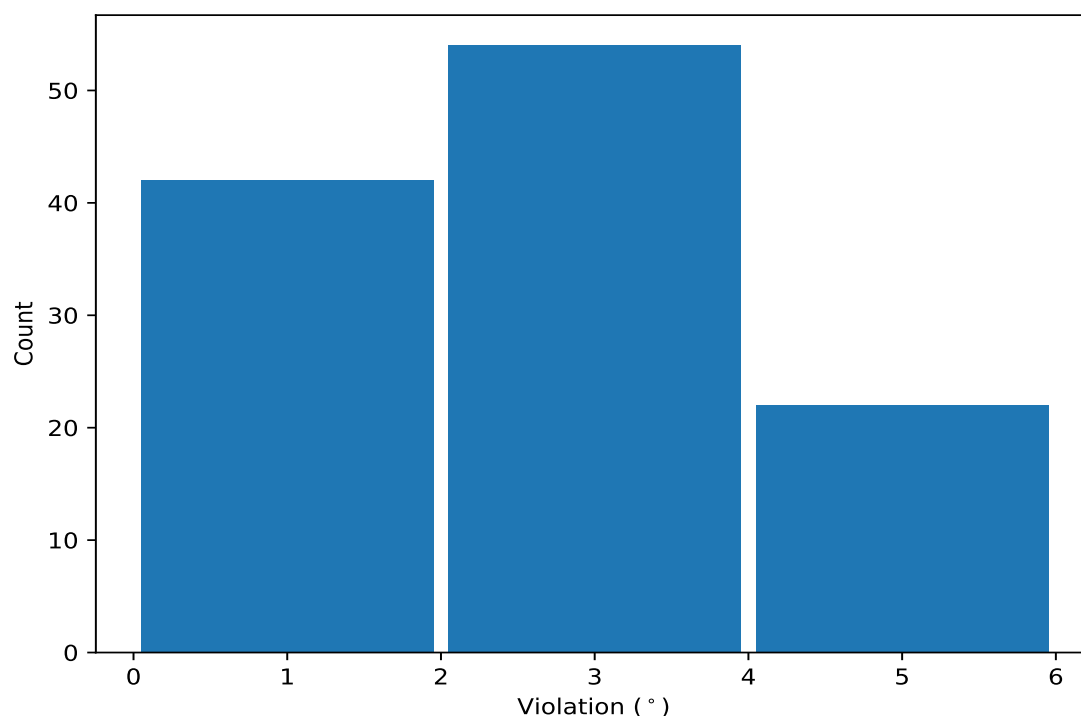
| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,124) | 1:75:A:LYS:N | 1:75:A:LYS:CA | 1:75:A:LYS:C  | 1:76:A:LYS:N | 2                   | 2.58 | 0.99            | 2.58   |
| (1,54)  | 1:37:A:SER:N | 1:37:A:SER:CA | 1:37:A:SER:C  | 1:38:A:SER:N | 2                   | 2.32 | 1.06            | 2.32   |
| (1,102) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C  | 1:64:A:LYS:N | 2                   | 2.16 | 0.9             | 2.16   |
| (1,97)  | 1:60:A:ASP:C | 1:61:A:VAL:N  | 1:61:A:VAL:CA | 1:61:A:VAL:C | 2                   | 2.0  | 0.69            | 2.0    |
| (1,48)  | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C  | 1:35:A:VAL:N | 2                   | 1.85 | 0.72            | 1.85   |
| (1,62)  | 1:41:A:LYS:N | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:TYR:N | 2                   | 1.77 | 0.19            | 1.77   |
| (1,143) | 1:84:A:LEU:C | 1:85:A:ILE:N  | 1:85:A:ILE:CA | 1:85:A:ILE:C | 2                   | 1.7  | 0.6             | 1.7    |
| (1,106) | 1:66:A:LYS:N | 1:66:A:LYS:CA | 1:66:A:LYS:C  | 1:67:A:ASN:N | 2                   | 1.58 | 0.24            | 1.58   |
| (1,142) | 1:84:A:LEU:N | 1:84:A:LEU:CA | 1:84:A:LEU:C  | 1:85:A:ILE:N | 2                   | 1.3  | 0.17            | 1.3    |

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

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

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

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



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

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

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 6        | 4.92          |
| (1,87)  | 1:55:A:GLY:C | 1:56:A:LYS:N  | 1:56:A:LYS:CA | 1:56:A:LYS:C | 10       | 4.92          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 2        | 4.91          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 20       | 4.89          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 47       | 4.86          |
| (1,66)  | 1:45:A:THR:N | 1:45:A:THR:CA | 1:45:A:THR:C  | 1:46:A:LYS:N | 40       | 4.84          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 5        | 4.78          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 7        | 4.78          |
| (1,71)  | 1:47:A:GLU:C | 1:48:A:ALA:N  | 1:48:A:ALA:CA | 1:48:A:ALA:C | 23       | 4.66          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 5        | 4.57          |
| (1,76)  | 1:50:A:GLU:N | 1:50:A:GLU:CA | 1:50:A:GLU:C  | 1:51:A:GLU:N | 14       | 4.5           |
| (1,141) | 1:83:A:LYS:C | 1:84:A:LEU:N  | 1:84:A:LEU:CA | 1:84:A:LEU:C | 40       | 4.48          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 24       | 4.47          |
| (1,71)  | 1:47:A:GLU:C | 1:48:A:ALA:N  | 1:48:A:ALA:CA | 1:48:A:ALA:C | 33       | 4.44          |
| (1,20)  | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C  | 1:18:A:GLN:N | 35       | 4.44          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 42       | 4.28          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 1        | 4.27          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 33       | 4.17          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 18       | 4.13          |
| (1,21)  | 1:17:A:LEU:C | 1:18:A:GLN:N  | 1:18:A:GLN:CA | 1:18:A:GLN:C | 37       | 4.12          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 38       | 4.07          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 30       | 4.0           |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 16       | 3.9           |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 12       | 3.85          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 17       | 3.85          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 4        | 3.81          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 11       | 3.81          |
| (1,139) | 1:82:A:GLN:C | 1:83:A:LYS:N  | 1:83:A:LYS:CA | 1:83:A:LYS:C | 35       | 3.73          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 24       | 3.7           |
| (1,66)  | 1:45:A:THR:N | 1:45:A:THR:CA | 1:45:A:THR:C  | 1:46:A:LYS:N | 23       | 3.69          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 7        | 3.68          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 22       | 3.68          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 9        | 3.63          |
| (1,87)  | 1:55:A:GLY:C | 1:56:A:LYS:N  | 1:56:A:LYS:CA | 1:56:A:LYS:C | 5        | 3.61          |
| (1,124) | 1:75:A:LYS:N | 1:75:A:LYS:CA | 1:75:A:LYS:C  | 1:76:A:LYS:N | 48       | 3.57          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 4        | 3.55          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 48       | 3.55          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 12       | 3.5           |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 27       | 3.48          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 1        | 3.42          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 39       | 3.41          |
| (1,54)  | 1:37:A:SER:N | 1:37:A:SER:CA | 1:37:A:SER:C  | 1:38:A:SER:N | 38       | 3.38          |
| (1,16)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:LEU:N | 40       | 3.38          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 17       | 3.37          |
| (1,103) | 1:63:A:LYS:C | 1:64:A:LYS:N  | 1:64:A:LYS:CA | 1:64:A:LYS:C | 19       | 3.33          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 21       | 3.29          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 20       | 3.28          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 18       | 3.21          |
| (1,82)  | 1:53:A:ARG:N | 1:53:A:ARG:CA | 1:53:A:ARG:C  | 1:54:A:LEU:N | 5        | 3.15          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 13       | 3.13          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 8        | 3.1           |
| (1,102) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C  | 1:64:A:LYS:N | 22       | 3.06          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,87)  | 1:55:A:GLY:C | 1:56:A:LYS:N  | 1:56:A:LYS:CA | 1:56:A:LYS:C | 27       | 3.05          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 40       | 3.01          |
| (1,7)   | 1:10:A:GLN:C | 1:11:A:GLN:N  | 1:11:A:GLN:CA | 1:11:A:GLN:C | 45       | 2.97          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 8        | 2.94          |
| (1,144) | 1:85:A:ILE:N | 1:85:A:ILE:CA | 1:85:A:ILE:C  | 1:86:A:GLU:N | 19       | 2.93          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 37       | 2.92          |
| (1,82)  | 1:53:A:ARG:N | 1:53:A:ARG:CA | 1:53:A:ARG:C  | 1:54:A:LEU:N | 12       | 2.78          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 44       | 2.75          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 39       | 2.71          |
| (1,97)  | 1:60:A:ASP:C | 1:61:A:VAL:N  | 1:61:A:VAL:CA | 1:61:A:VAL:C | 46       | 2.69          |
| (1,16)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:LEU:N | 25       | 2.66          |
| (1,87)  | 1:55:A:GLY:C | 1:56:A:LYS:N  | 1:56:A:LYS:CA | 1:56:A:LYS:C | 21       | 2.65          |
| (1,1)   | 1:6:A:PRO:C  | 1:7:A:ALA:N   | 1:7:A:ALA:CA  | 1:7:A:ALA:C  | 25       | 2.61          |
| (1,48)  | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C  | 1:35:A:VAL:N | 26       | 2.57          |
| (1,87)  | 1:55:A:GLY:C | 1:56:A:LYS:N  | 1:56:A:LYS:CA | 1:56:A:LYS:C | 18       | 2.55          |
| (1,7)   | 1:10:A:GLN:C | 1:11:A:GLN:N  | 1:11:A:GLN:CA | 1:11:A:GLN:C | 19       | 2.46          |
| (1,103) | 1:63:A:LYS:C | 1:64:A:LYS:N  | 1:64:A:LYS:CA | 1:64:A:LYS:C | 35       | 2.37          |
| (1,87)  | 1:55:A:GLY:C | 1:56:A:LYS:N  | 1:56:A:LYS:CA | 1:56:A:LYS:C | 12       | 2.31          |
| (1,143) | 1:84:A:LEU:C | 1:85:A:ILE:N  | 1:85:A:ILE:CA | 1:85:A:ILE:C | 25       | 2.29          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 35       | 2.28          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 4        | 2.28          |
| (1,144) | 1:85:A:ILE:N | 1:85:A:ILE:CA | 1:85:A:ILE:C  | 1:86:A:GLU:N | 40       | 2.24          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 14       | 2.12          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 9        | 2.03          |
| (1,62)  | 1:41:A:LYS:N | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:TYR:N | 21       | 1.96          |
| (1,87)  | 1:55:A:GLY:C | 1:56:A:LYS:N  | 1:56:A:LYS:CA | 1:56:A:LYS:C | 4        | 1.93          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 23       | 1.92          |
| (1,139) | 1:82:A:GLN:C | 1:83:A:LYS:N  | 1:83:A:LYS:CA | 1:83:A:LYS:C | 41       | 1.83          |
| (1,106) | 1:66:A:LYS:N | 1:66:A:LYS:CA | 1:66:A:LYS:C  | 1:67:A:ASN:N | 44       | 1.83          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 18       | 1.83          |
| (1,104) | 1:64:A:LYS:N | 1:64:A:LYS:CA | 1:64:A:LYS:C  | 1:65:A:THR:N | 28       | 1.78          |
| (1,7)   | 1:10:A:GLN:C | 1:11:A:GLN:N  | 1:11:A:GLN:CA | 1:11:A:GLN:C | 25       | 1.75          |
| (1,139) | 1:82:A:GLN:C | 1:83:A:LYS:N  | 1:83:A:LYS:CA | 1:83:A:LYS:C | 40       | 1.73          |
| (1,144) | 1:85:A:ILE:N | 1:85:A:ILE:CA | 1:85:A:ILE:C  | 1:86:A:GLU:N | 12       | 1.7           |
| (1,7)   | 1:10:A:GLN:C | 1:11:A:GLN:N  | 1:11:A:GLN:CA | 1:11:A:GLN:C | 31       | 1.7           |
| (1,7)   | 1:10:A:GLN:C | 1:11:A:GLN:N  | 1:11:A:GLN:CA | 1:11:A:GLN:C | 34       | 1.68          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 28       | 1.62          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 31       | 1.62          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 30       | 1.61          |
| (1,124) | 1:75:A:LYS:N | 1:75:A:LYS:CA | 1:75:A:LYS:C  | 1:76:A:LYS:N | 29       | 1.58          |
| (1,62)  | 1:41:A:LYS:N | 1:41:A:LYS:CA | 1:41:A:LYS:C  | 1:42:A:TYR:N | 40       | 1.58          |
| (1,16)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:LEU:N | 30       | 1.58          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 16       | 1.54          |
| (1,144) | 1:85:A:ILE:N | 1:85:A:ILE:CA | 1:85:A:ILE:C  | 1:86:A:GLU:N | 28       | 1.52          |
| (1,142) | 1:84:A:LEU:N | 1:84:A:LEU:CA | 1:84:A:LEU:C  | 1:85:A:ILE:N | 47       | 1.47          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 25       | 1.43          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 9        | 1.4           |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 37       | 1.4           |
| (1,65)  | 1:44:A:ILE:C | 1:45:A:THR:N  | 1:45:A:THR:CA | 1:45:A:THR:C | 36       | 1.4           |
| (1,106) | 1:66:A:LYS:N | 1:66:A:LYS:CA | 1:66:A:LYS:C  | 1:67:A:ASN:N | 47       | 1.34          |
| (1,97)  | 1:60:A:ASP:C | 1:61:A:VAL:N  | 1:61:A:VAL:CA | 1:61:A:VAL:C | 19       | 1.31          |

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*Continued from previous page...*

| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,16)  | 1:15:A:ARG:N | 1:15:A:ARG:CA | 1:15:A:ARG:C  | 1:16:A:LEU:N | 9        | 1.28          |
| (1,6)   | 1:10:A:GLN:N | 1:10:A:GLN:CA | 1:10:A:GLN:C  | 1:11:A:GLN:N | 34       | 1.28          |
| (1,102) | 1:63:A:LYS:N | 1:63:A:LYS:CA | 1:63:A:LYS:C  | 1:64:A:LYS:N | 28       | 1.25          |
| (1,54)  | 1:37:A:SER:N | 1:37:A:SER:CA | 1:37:A:SER:C  | 1:38:A:SER:N | 21       | 1.25          |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 22       | 1.24          |
| (1,67)  | 1:45:A:THR:C | 1:46:A:LYS:N  | 1:46:A:LYS:CA | 1:46:A:LYS:C | 7        | 1.23          |
| (1,95)  | 1:59:A:ASN:C | 1:60:A:ASP:N  | 1:60:A:ASP:CA | 1:60:A:ASP:C | 39       | 1.21          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 13       | 1.15          |
| (1,48)  | 1:34:A:GLU:N | 1:34:A:GLU:CA | 1:34:A:GLU:C  | 1:35:A:VAL:N | 9        | 1.13          |
| (1,142) | 1:84:A:LEU:N | 1:84:A:LEU:CA | 1:84:A:LEU:C  | 1:85:A:ILE:N | 48       | 1.12          |
| (1,143) | 1:84:A:LEU:C | 1:85:A:ILE:N  | 1:85:A:ILE:CA | 1:85:A:ILE:C | 42       | 1.1           |
| (1,72)  | 1:48:A:ALA:N | 1:48:A:ALA:CA | 1:48:A:ALA:C  | 1:49:A:LEU:N | 42       | 1.07          |
| (1,144) | 1:85:A:ILE:N | 1:85:A:ILE:CA | 1:85:A:ILE:C  | 1:86:A:GLU:N | 46       | 1.06          |
| (1,32)  | 1:24:A:SER:N | 1:24:A:SER:CA | 1:24:A:SER:C  | 1:25:A:ASN:N | 21       | 1.05          |
| (1,71)  | 1:47:A:GLU:C | 1:48:A:ALA:N  | 1:48:A:ALA:CA | 1:48:A:ALA:C | 30       | 1.0           |