



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 08:49 AM UTC

PDB ID : 6EMR / pdb\_00006emr  
BMRB ID : 34182  
Title : Solution structure of the LEDGF/p75 IBD - IWS1 (aa 446-548) complex  
Authors : Veverka, V.  
Deposited on : 2017-10-03

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

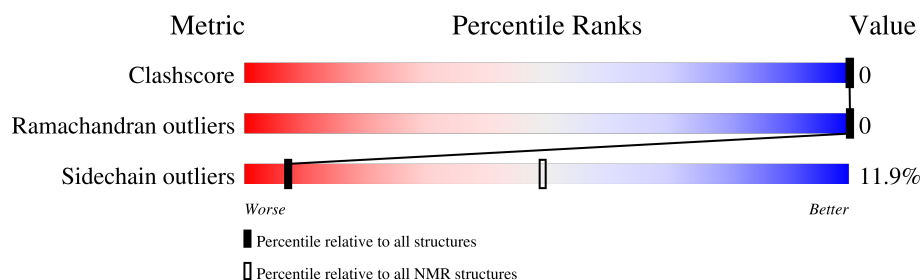
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 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     | 206    |  |

## 2 Ensemble composition and analysis

This entry contains 40 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                                            |                   |              |
|--------------------------------------|--------------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)                      | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:348-A:428, A:472-A:477, A:489-A:496 (95) | 0.38              | 13           |
| 2                                    | A:529-A:538 (10)                           | 0.23              | 20           |

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 8 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3278 atoms, of which 1616 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PC4 and SFRS1-interacting protein, Protein IWS1 homolog.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|-------|
| 1   | A     | 206      | Total | C    | H    | N   | O   | S  | 0     |
|     |       |          | 3278  | 1011 | 1616 | 289 | 351 | 11 |       |

There are 6 discrepancies between the modelled and reference sequences:

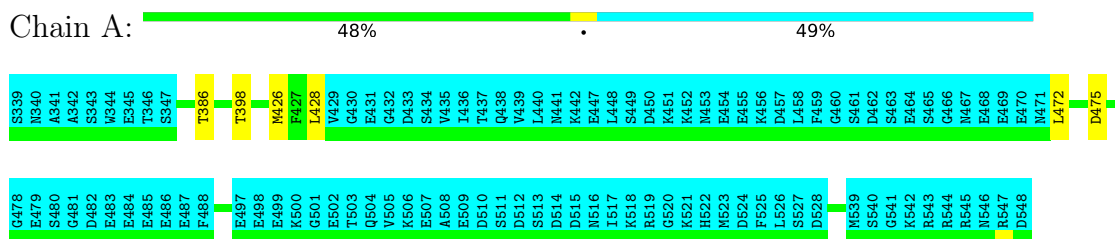
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 339     | SER      | -      | expression tag | UNP O75475 |
| A     | 340     | ASN      | -      | expression tag | UNP O75475 |
| A     | 341     | ALA      | -      | expression tag | UNP O75475 |
| A     | 342     | ALA      | -      | expression tag | UNP O75475 |
| A     | 343     | SER      | -      | expression tag | UNP O75475 |
| A     | 344     | TRP      | -      | expression tag | UNP O75475 |

## 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: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

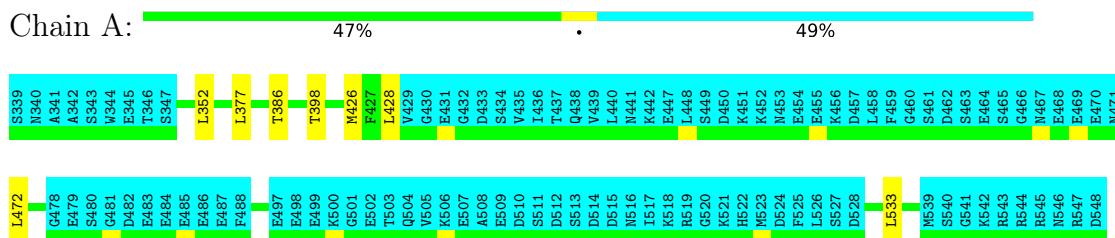


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

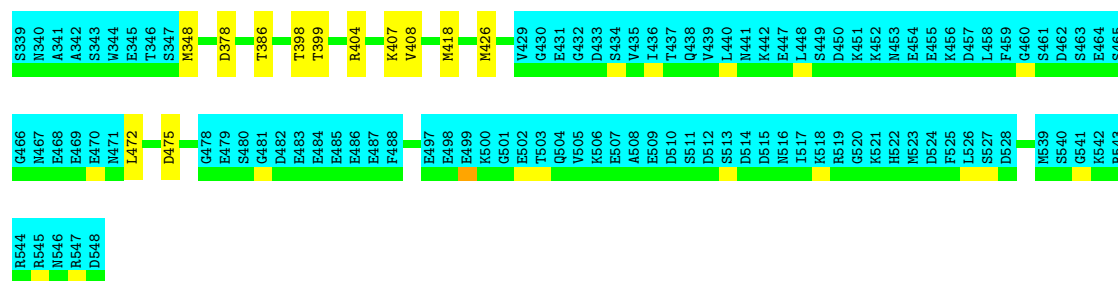
- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



#### 4.2.2 Score per residue for model 2

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

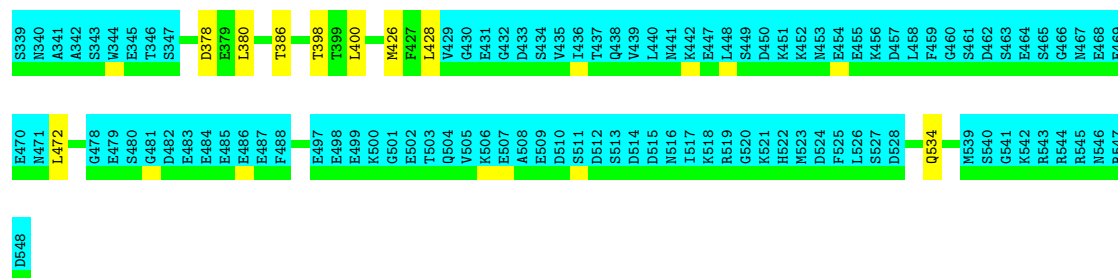




#### 4.2.3 Score per residue for model 3

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

Chain A: 47% . 49%



#### 4.2.4 Score per residue for model 4

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

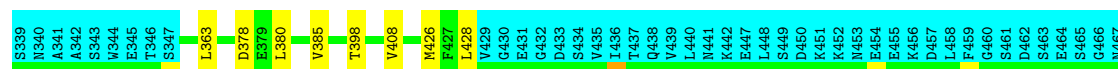
Chain A: 45% 6% 49%

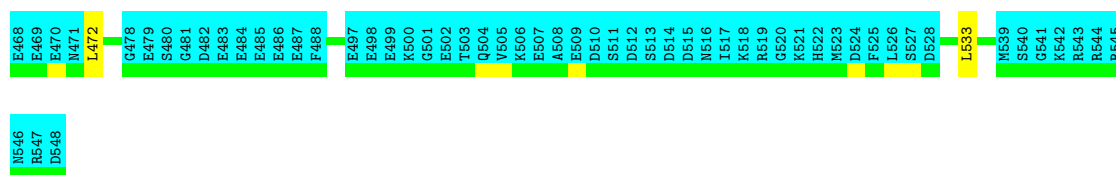


#### 4.2.5 Score per residue for model 5

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

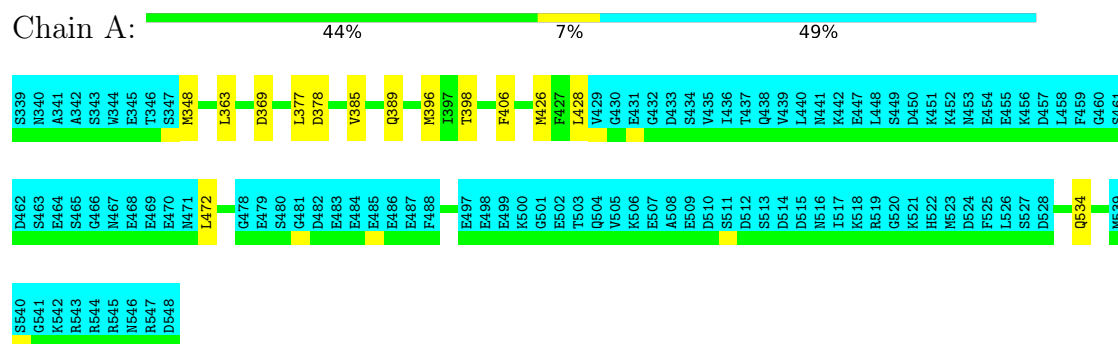
Chain A: 46% 5% 49%





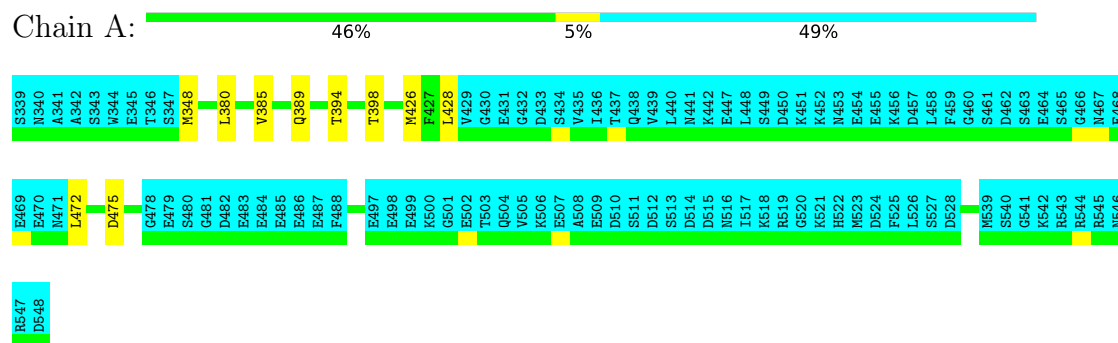
#### 4.2.6 Score per residue for model 6

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



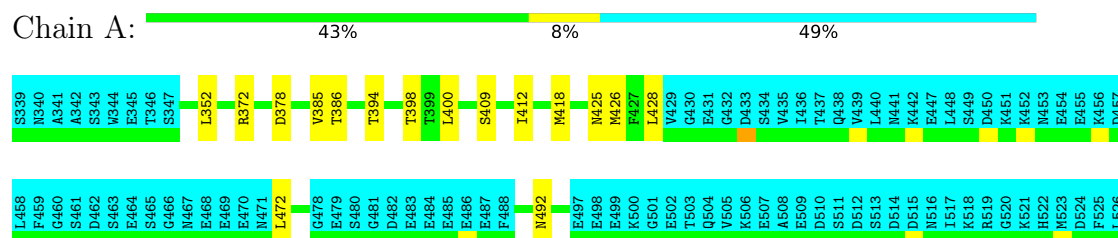
#### 4.2.7 Score per residue for model 7

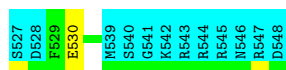
- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



#### 4.2.8 Score per residue for model 8

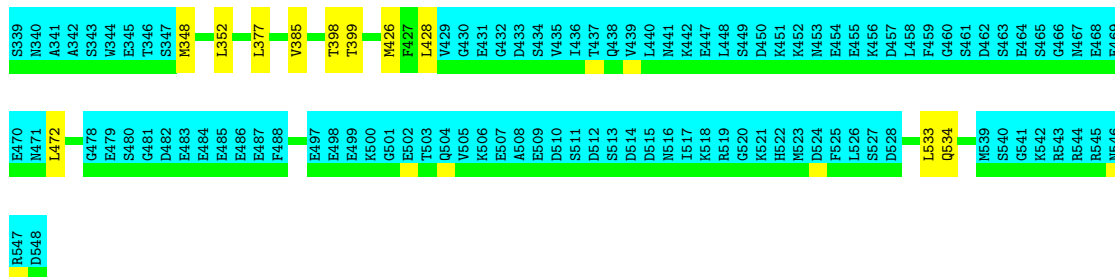
- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog





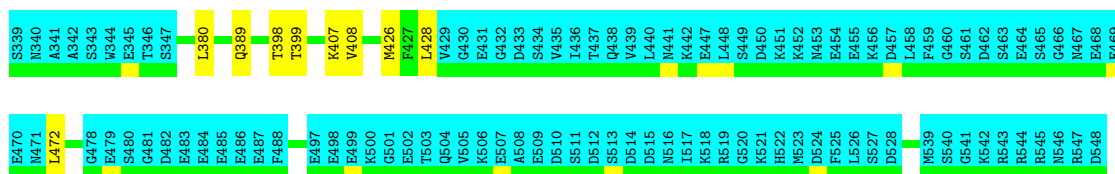
#### 4.2.9 Score per residue for model 9

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



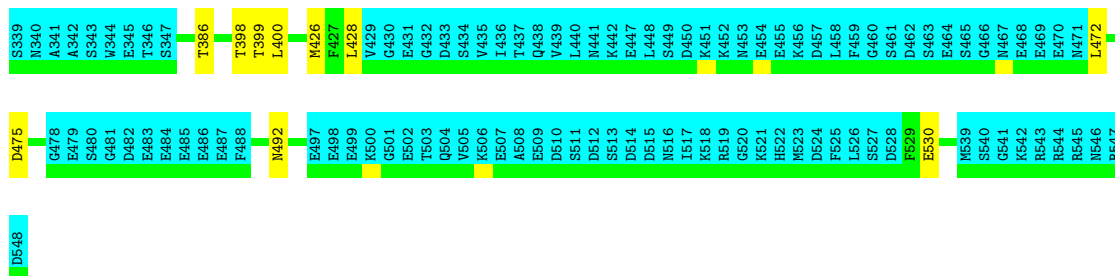
#### 4.2.10 Score per residue for model 10

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



#### 4.2.11 Score per residue for model 11

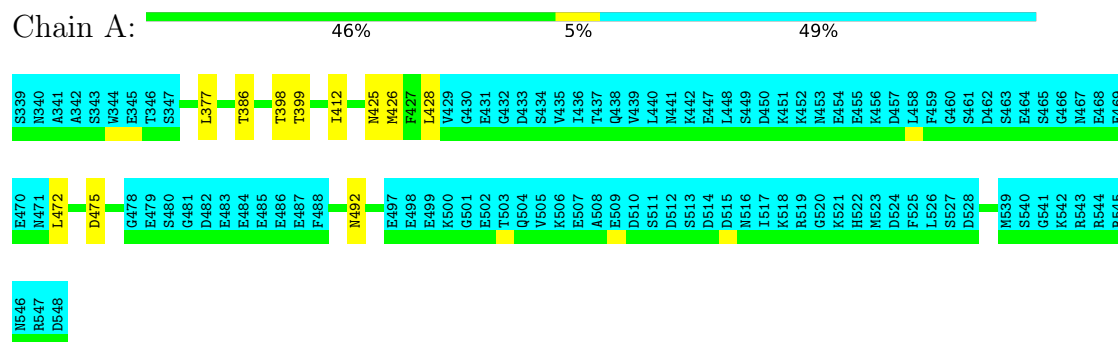
- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog





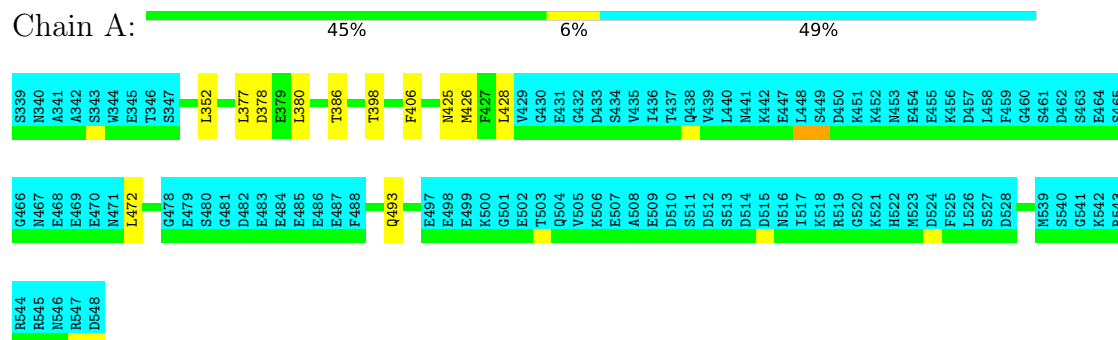
### 4.2.15 Score per residue for model 15

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



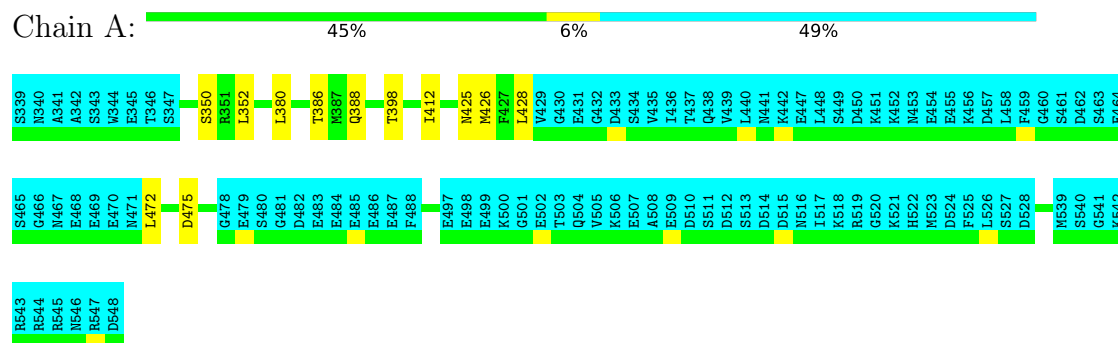
### 4.2.16 Score per residue for model 16

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



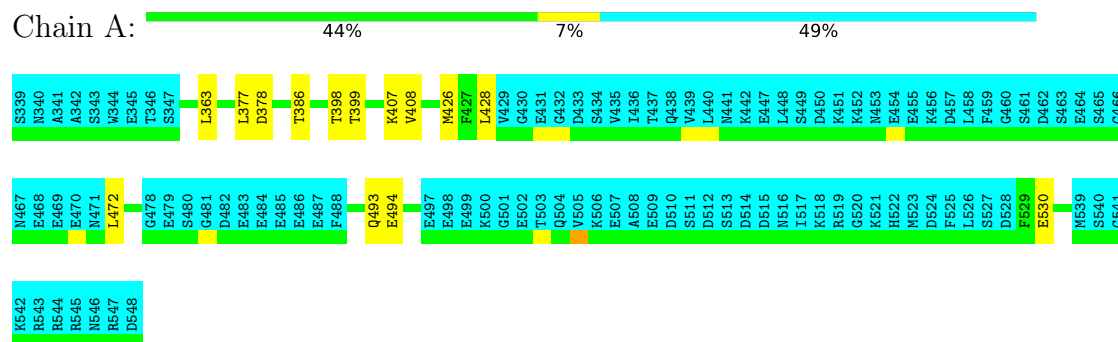
### 4.2.17 Score per residue for model 17

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



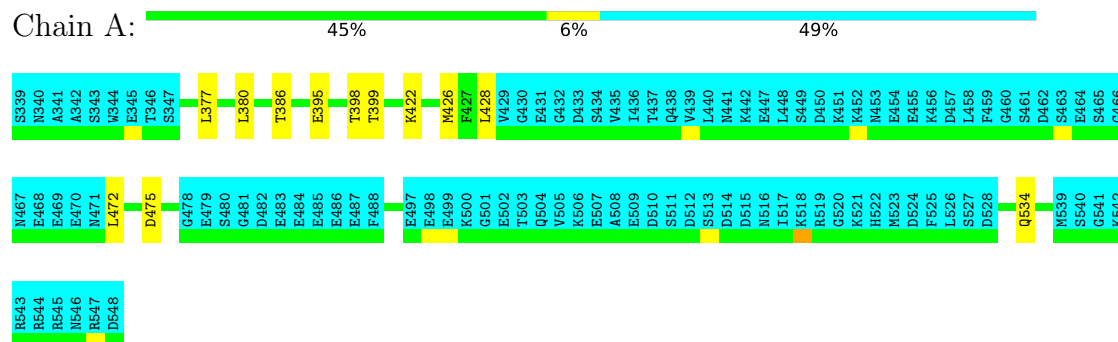
### 4.2.18 Score per residue for model 18

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



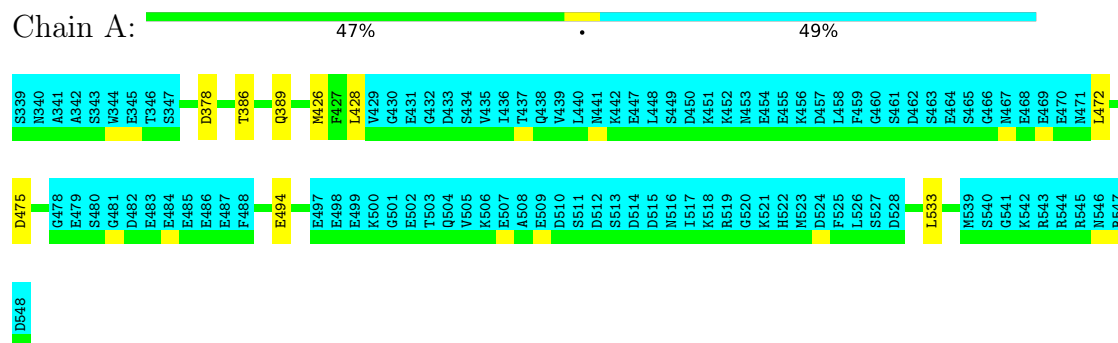
### 4.2.19 Score per residue for model 19

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



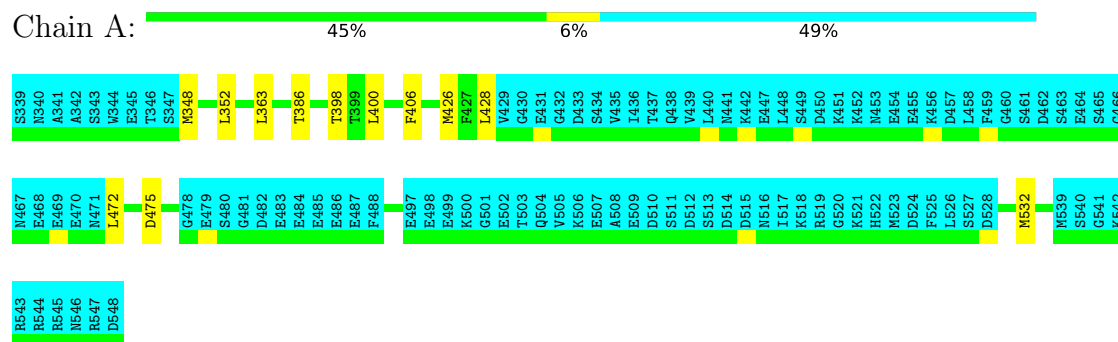
### 4.2.20 Score per residue for model 20

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



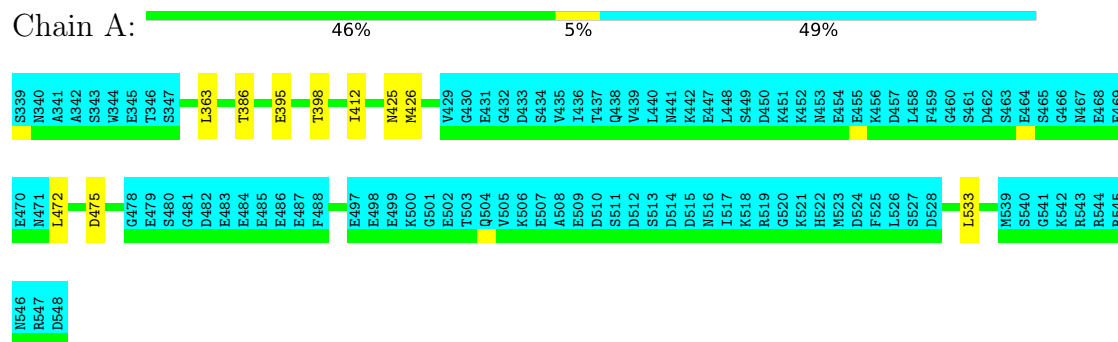
### 4.2.21 Score per residue for model 21

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



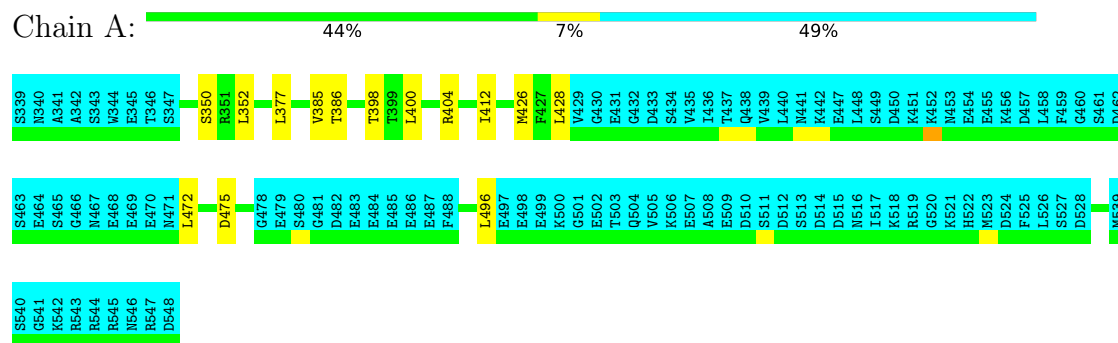
### 4.2.22 Score per residue for model 22

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



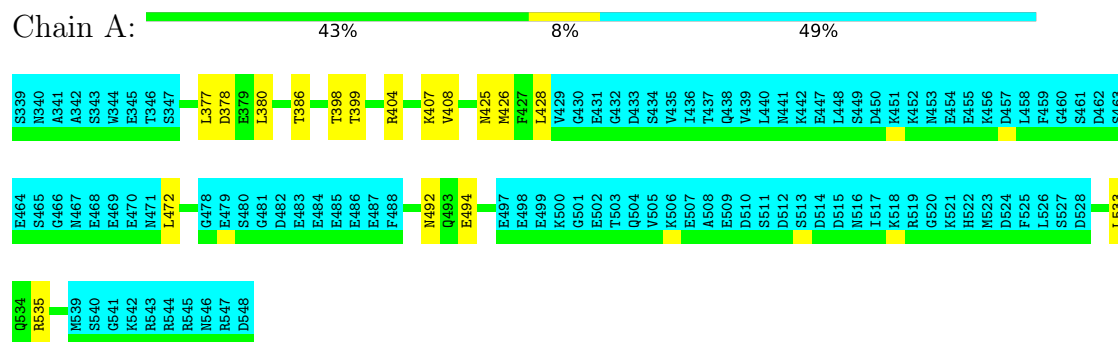
### 4.2.23 Score per residue for model 23

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



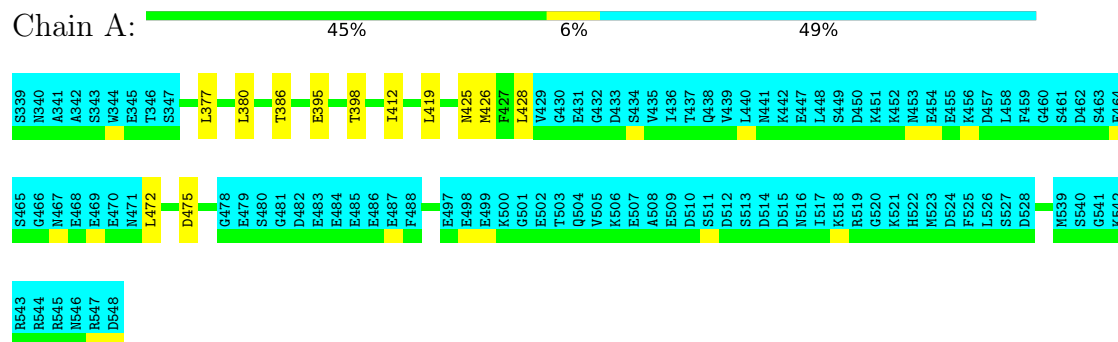
### 4.2.24 Score per residue for model 24

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



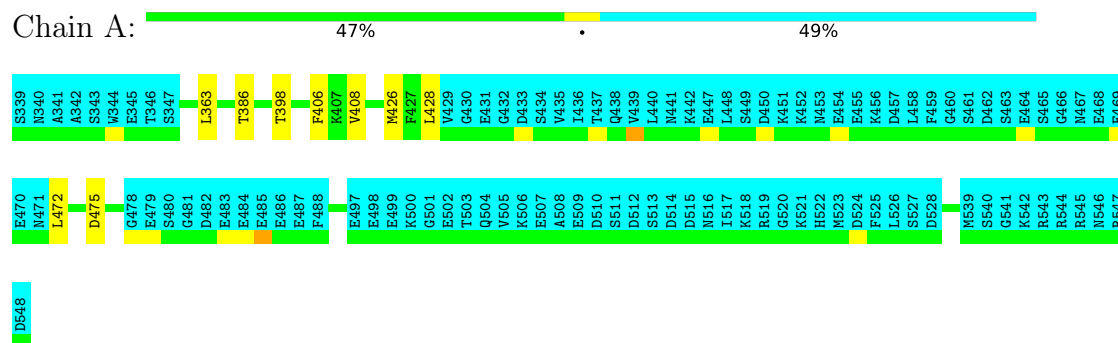
### 4.2.25 Score per residue for model 25

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



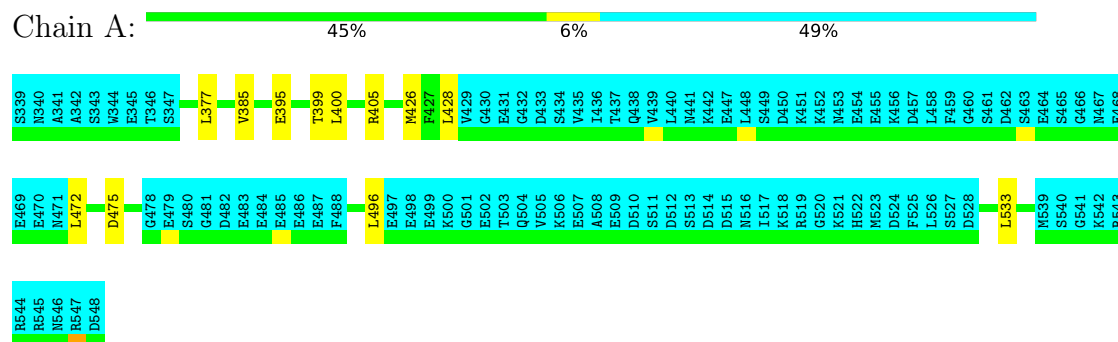
### 4.2.26 Score per residue for model 26

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



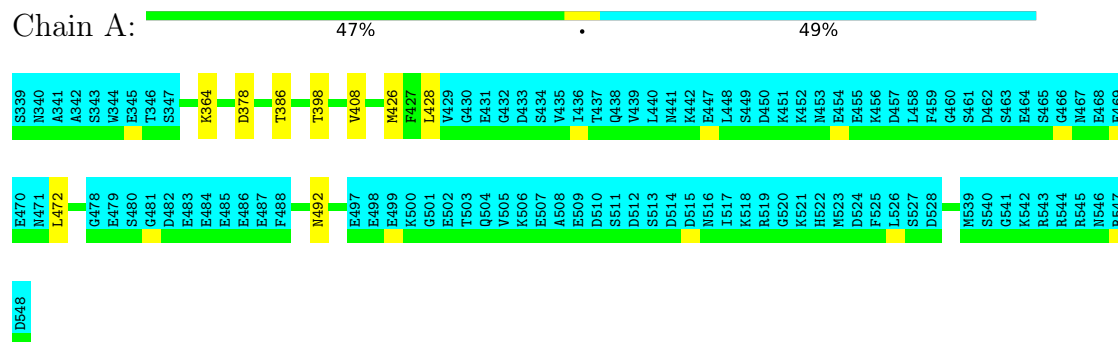
### 4.2.27 Score per residue for model 27

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



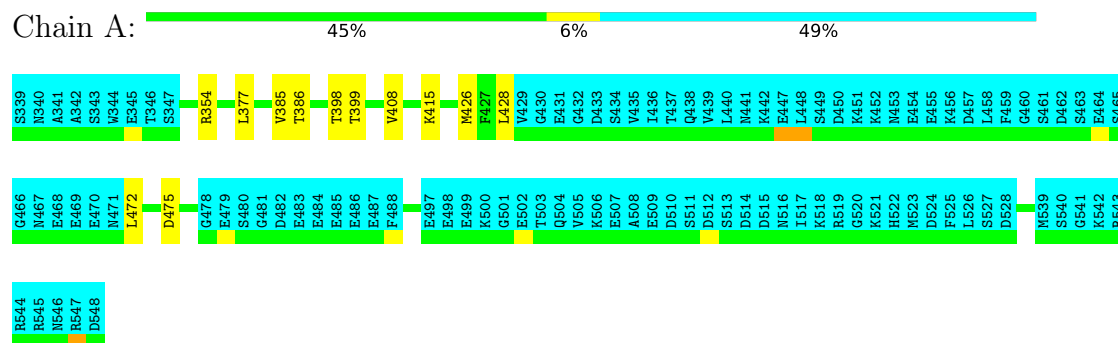
### 4.2.28 Score per residue for model 28

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



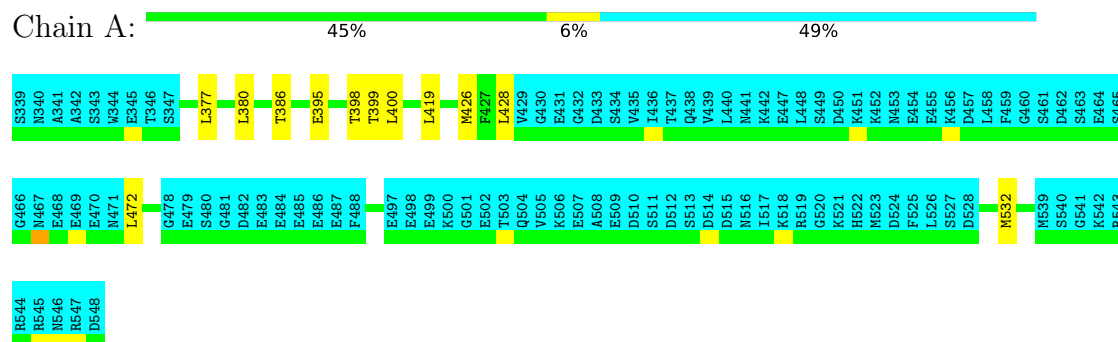
### 4.2.29 Score per residue for model 29

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



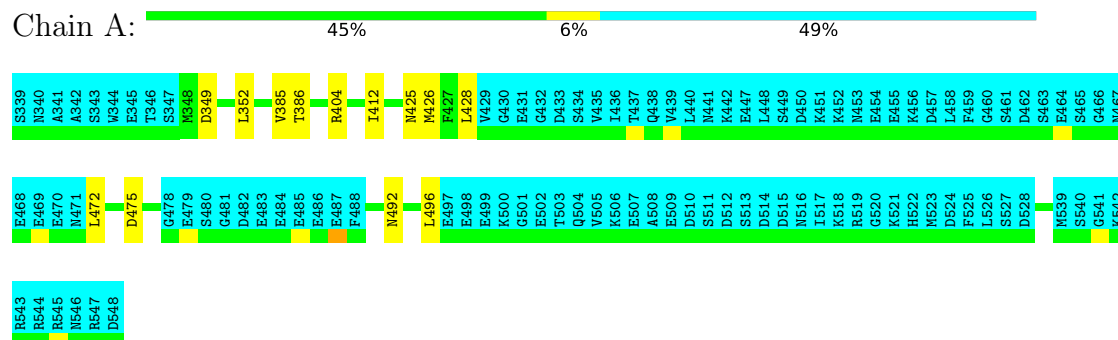
### 4.2.30 Score per residue for model 30

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



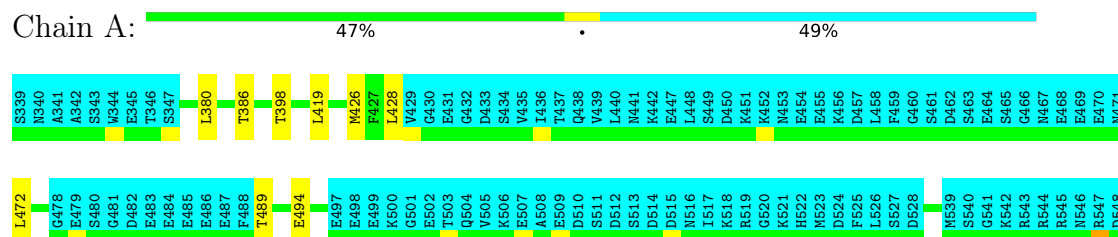
### 4.2.31 Score per residue for model 31

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



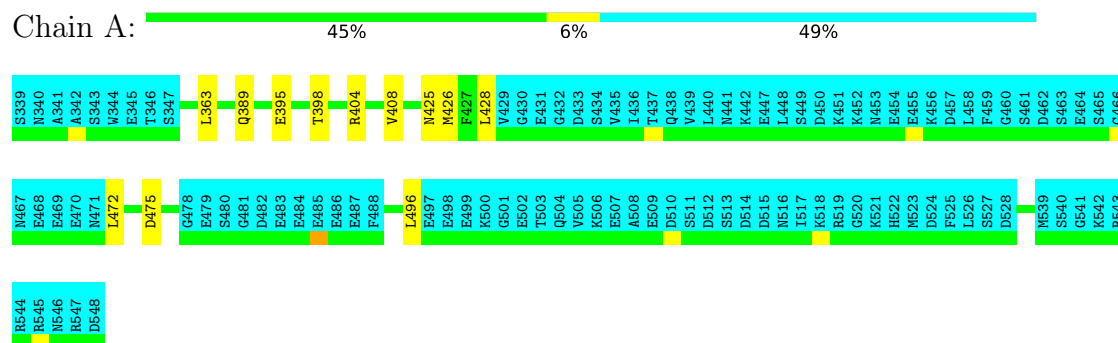
### 4.2.32 Score per residue for model 32

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



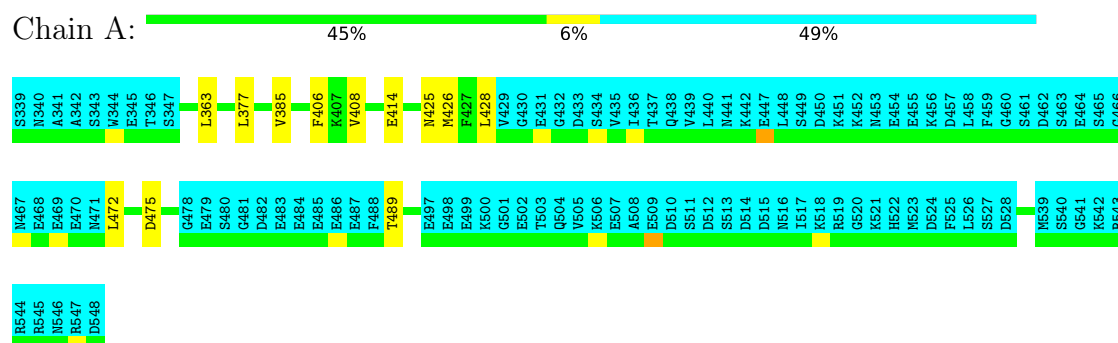
### 4.2.33 Score per residue for model 33

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



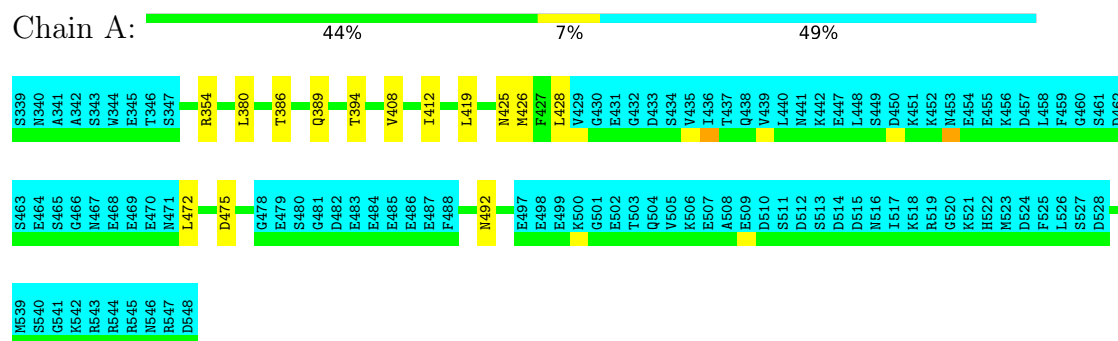
#### 4.2.34 Score per residue for model 34

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



#### 4.2.35 Score per residue for model 35

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



#### 4.2.36 Score per residue for model 36

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

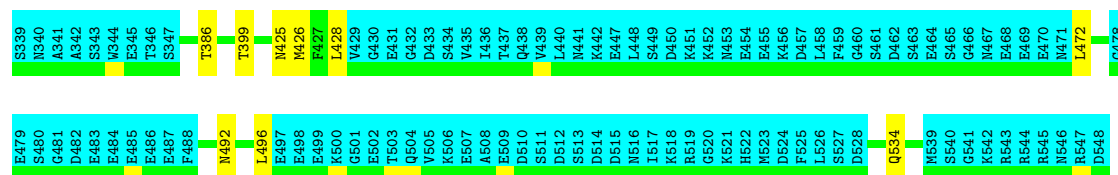




#### 4.2.37 Score per residue for model 37

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

Chain A: 47% . 49%



#### 4.2.38 Score per residue for model 38

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

Chain A: 44% 7% 49%

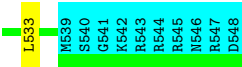


#### 4.2.39 Score per residue for model 39

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog

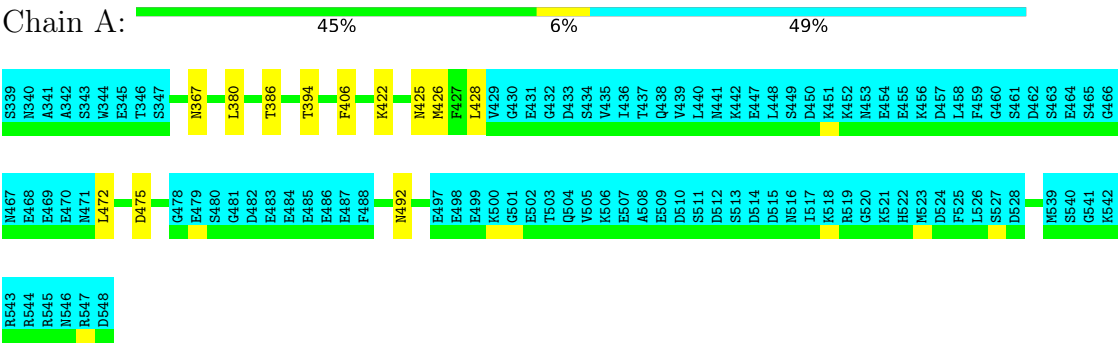
Chain A: 43% 8% 49%





4.2.40 Score per residue for model 40

- Molecule 1: PC4 and SFRS1-interacting protein,Protein IWS1 homolog



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 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 |
|---------------|--------------------|---------|
| TopSpin       | refinement         |         |
| Sparky        | structure solution |         |
| CYANA         | structure solution |         |

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                       | 2407           |
| Number of shifts mapped to atoms             | 2407           |
| 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     | 0.76±0.02    | 0±0/876 ( 0.0± 0.0%) | 0.88±0.02   | 0±0/1168 ( 0.0± 0.0%) |
| All | All   | 0.76         | 0/35040 ( 0.0%)      | 0.88        | 10/46720 ( 0.0%)      |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 386 | THR  | N-CA-C | -5.69 | 102.10      | 110.52   | 29     | 4     |
| 1   | A     | 407 | LYS  | N-CA-C | 5.65  | 118.98      | 111.75   | 10     | 5     |
| 1   | A     | 404 | ARG  | N-CA-C | -5.18 | 105.81      | 111.82   | 33     | 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     | 867   | 908      | 908      | 0±0     |
| All | All   | 34680 | 36320    | 36320    | 1       |

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:406:PHE:CD2 | 1:A:408:VAL:HG22 | 0.41     | 2.51        | 26     | 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     | 105/206 (51%)   | 101±1 (97±1%) | 4±1 (3±1%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 4200/8240 (51%) | 4058 (97%)    | 142 (3%)   | 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     | 99/188 (53%)    | 87±3 (88±3%) | 12±3 (12±3%) | 7           | 49 |
| All | All   | 3960/7520 (53%) | 3490 (88%)   | 470 (12%)    | 7           | 49 |

All 52 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     | 426 | MET  | 40             |
| 1   | A     | 472 | LEU  | 40             |
| 1   | A     | 428 | LEU  | 35             |
| 1   | A     | 398 | THR  | 32             |
| 1   | A     | 386 | THR  | 26             |
| 1   | A     | 475 | ASP  | 24             |
| 1   | A     | 380 | LEU  | 17             |
| 1   | A     | 377 | LEU  | 16             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 385 | VAL  | 16             |
| 1   | A     | 399 | THR  | 14             |
| 1   | A     | 408 | VAL  | 14             |
| 1   | A     | 425 | ASN  | 14             |
| 1   | A     | 400 | LEU  | 13             |
| 1   | A     | 412 | ILE  | 12             |
| 1   | A     | 378 | ASP  | 11             |
| 1   | A     | 395 | GLU  | 11             |
| 1   | A     | 533 | LEU  | 10             |
| 1   | A     | 363 | LEU  | 10             |
| 1   | A     | 352 | LEU  | 9              |
| 1   | A     | 492 | ASN  | 9              |
| 1   | A     | 419 | LEU  | 8              |
| 1   | A     | 406 | PHE  | 7              |
| 1   | A     | 496 | LEU  | 7              |
| 1   | A     | 389 | GLN  | 6              |
| 1   | A     | 494 | GLU  | 6              |
| 1   | A     | 348 | MET  | 5              |
| 1   | A     | 404 | ARG  | 5              |
| 1   | A     | 534 | GLN  | 5              |
| 1   | A     | 394 | THR  | 4              |
| 1   | A     | 530 | GLU  | 4              |
| 1   | A     | 493 | GLN  | 4              |
| 1   | A     | 349 | ASP  | 3              |
| 1   | A     | 489 | THR  | 3              |
| 1   | A     | 418 | MET  | 2              |
| 1   | A     | 369 | ASP  | 2              |
| 1   | A     | 372 | ARG  | 2              |
| 1   | A     | 351 | ARG  | 2              |
| 1   | A     | 350 | SER  | 2              |
| 1   | A     | 422 | LYS  | 2              |
| 1   | A     | 532 | MET  | 2              |
| 1   | A     | 405 | ARG  | 2              |
| 1   | A     | 364 | LYS  | 2              |
| 1   | A     | 354 | ARG  | 2              |
| 1   | A     | 415 | LYS  | 2              |
| 1   | A     | 396 | MET  | 1              |
| 1   | A     | 409 | SER  | 1              |
| 1   | A     | 358 | GLU  | 1              |
| 1   | A     | 401 | LYS  | 1              |
| 1   | A     | 388 | GLN  | 1              |
| 1   | A     | 535 | ARG  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 414 | GLU  | 1              |
| 1   | A     | 367 | ASN  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 86% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *str\_nozero.str*

#### 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                  | 2407 |
| Number of shifts mapped to atoms        | 2407 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 4    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 202      | $-0.44 \pm 0.07$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 193      | $0.12 \pm 0.03$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 199      | $-0.34 \pm 0.03$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 199      | $-0.56 \pm 0.08$                | Should be applied          |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1382 atoms were assigned a chemical shift out of a possible 1552. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 509/526 (97%) | 206/211 (98%) | 203/210 (97%)   | 100/105 (95%)   |
| Sidechain | 819/943 (87%) | 564/610 (92%) | 244/290 (84%)   | 11/43 (26%)     |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 54/83 (65%)     | 34/42 (81%)    | 20/39 (51%)     | 0/2 (0%)        |
| Overall  | 1382/1552 (89%) | 804/863 (93%)  | 467/539 (87%)   | 111/150 (74%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 2402 atoms were assigned a chemical shift out of a possible 2808. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H  | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone  | 1011/1040 (97%) | 411/422 (97%)   | 401/412 (97%)   | 199/206 (97%)   |
| Sidechain | 1306/1636 (80%) | 875/1038 (84%)  | 417/522 (80%)   | 14/76 (18%)     |
| Aromatic  | 85/132 (64%)    | 52/67 (78%)     | 32/61 (52%)     | 1/4 (25%)       |
| Overall   | 2402/2808 (86%) | 1338/1527 (88%) | 850/995 (85%)   | 214/286 (75%)   |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

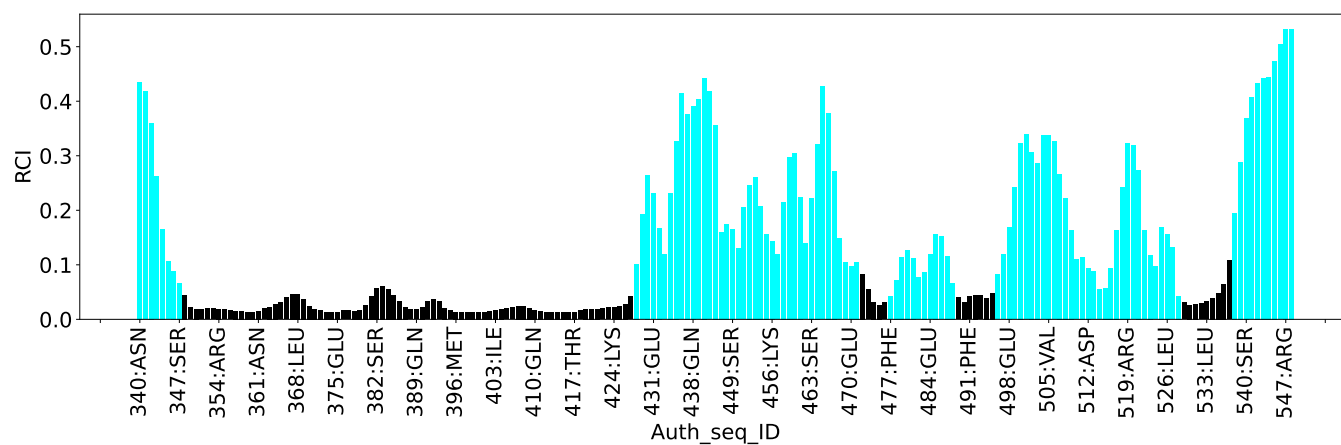
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 417 | THR  | HG1  | 5.67       | 0.08 – 2.19         | 21.5    |
| 1       | A     | 386 | THR  | HG1  | 5.57       | 0.08 – 2.19         | 21.0    |
| 1       | A     | 399 | THR  | HG1  | 3.00       | 0.08 – 2.19         | 8.8     |
| 1       | A     | 360 | LYS  | HE3  | 1.85       | 1.92 – 3.89         | -5.4    |

#### 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                                | 2841  |
| Intra-residue ( $ i-j =0$ )                              | 833   |
| Sequential ( $ i-j =1$ )                                 | 863   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 553   |
| Long range ( $ i-j \geq 5$ )                             | 592   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 226   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 14.9  |
| Number of long range restraints per residue <sup>1</sup> | 2.9   |

<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)  | 5.7                                    | 0.2     |
| 0.2-0.5 (Medium) | 1.9                                    | 0.5     |
| >0.5 (Large)     | 0.9                                    | 0.76    |

### 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)   | 2.1                                    | 5.87    |
| 10.0-20.0 (Medium) | 0.0                                    | 10.97   |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

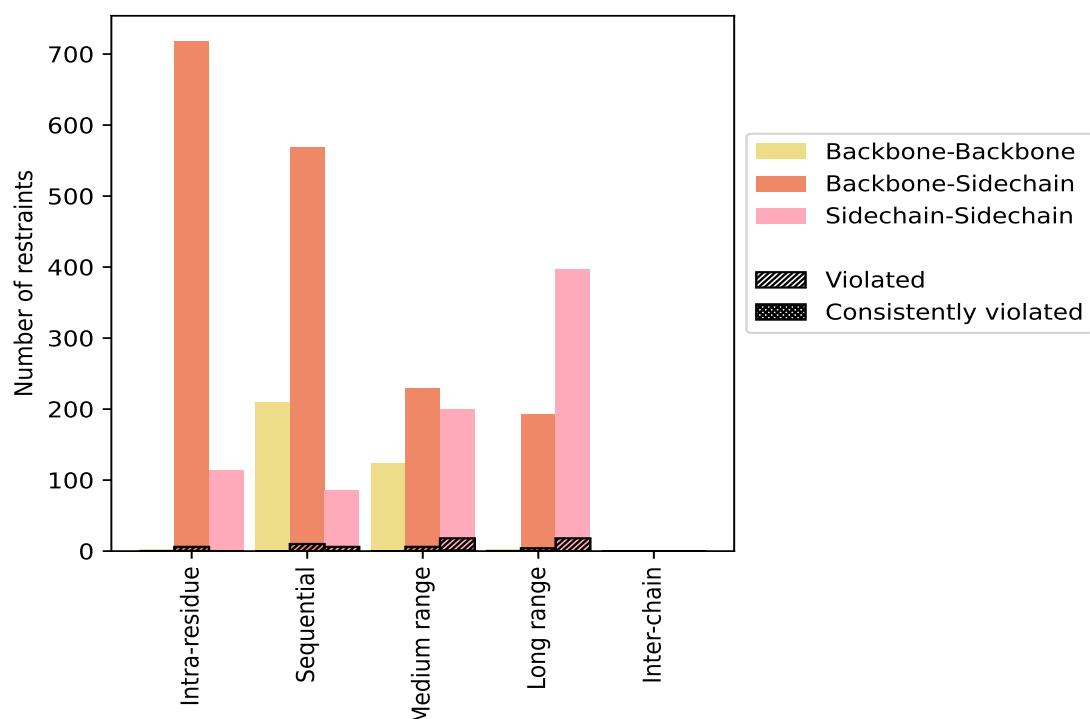
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>833</b>  | <b>29.3</b>    | <b>6</b>              | <b>0.7</b>     | <b>0.2</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 2           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 718         | 25.3           | 6                     | 0.8            | 0.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 113         | 4.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>863</b>  | <b>30.4</b>    | <b>16</b>             | <b>1.9</b>     | <b>0.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 210         | 7.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 568         | 20.0           | 10                    | 1.8            | 0.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 85          | 3.0            | 6                     | 7.1            | 0.2            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>553</b>  | <b>19.5</b>    | <b>24</b>             | <b>4.3</b>     | <b>0.8</b>     | <b>1</b>                           | <b>0.2</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 124         | 4.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 229         | 8.1            | 6                     | 2.6            | 0.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 200         | 7.0            | 18                    | 9.0            | 0.6            | 1                                  | 0.5            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>592</b>  | <b>20.8</b>    | <b>22</b>             | <b>3.7</b>     | <b>0.8</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 3           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 192         | 6.8            | 4                     | 2.1            | 0.1            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 397         | 14.0           | 18                    | 4.5            | 0.6            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>2841</b> | <b>100.0</b>   | <b>68</b>             | <b>2.4</b>     | <b>2.4</b>     | <b>1</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 339         | 11.9           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1707        | 60.1           | 26                    | 1.5            | 0.9            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 795         | 28.0           | 42                    | 5.3            | 1.5            | 1                                  | 0.1            | 0.0            |

<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        | 1                    | 3               | 3               | 4               | 0               | 11    | 0.18     | 0.36    | 0.07                | 0.14       |
| 2        | 0                    | 2               | 4               | 7               | 0               | 13    | 0.21     | 0.71    | 0.15                | 0.16       |
| 3        | 1                    | 2               | 6               | 4               | 0               | 13    | 0.22     | 0.76    | 0.17                | 0.16       |
| 4        | 1                    | 4               | 3               | 4               | 0               | 12    | 0.2      | 0.73    | 0.16                | 0.15       |
| 5        | 1                    | 5               | 4               | 5               | 0               | 15    | 0.22     | 0.71    | 0.14                | 0.19       |
| 6        | 1                    | 4               | 5               | 3               | 0               | 13    | 0.21     | 0.72    | 0.16                | 0.15       |
| 7        | 2                    | 0               | 3               | 1               | 0               | 6     | 0.24     | 0.7     | 0.21                | 0.16       |
| 8        | 1                    | 4               | 5               | 2               | 0               | 12    | 0.18     | 0.71    | 0.16                | 0.12       |
| 9        | 1                    | 1               | 7               | 6               | 0               | 15    | 0.2      | 0.72    | 0.15                | 0.15       |
| 10       | 1                    | 5               | 3               | 6               | 0               | 15    | 0.21     | 0.71    | 0.14                | 0.18       |

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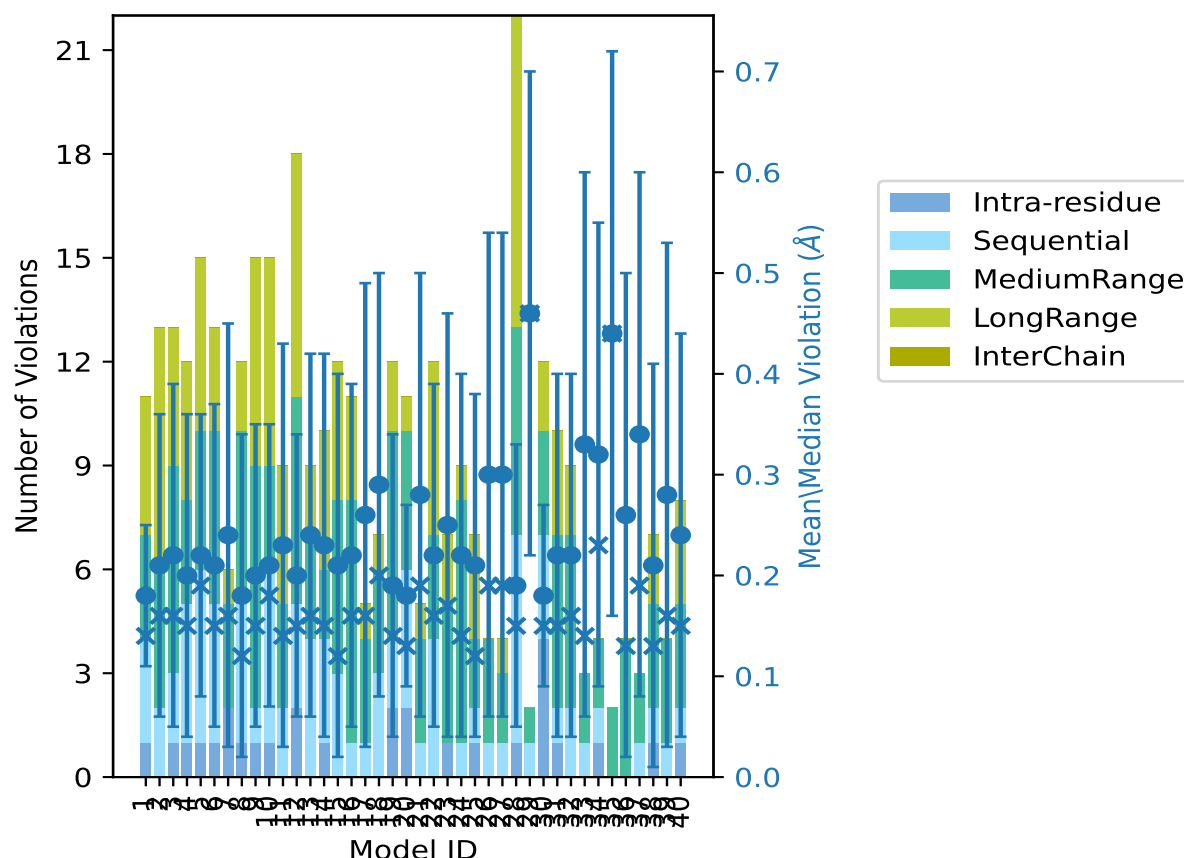
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 2               | 3               | 4               | 0               | 9     | 0.23     | 0.73    | 0.2                 | 0.14       |
| 12       | 2                    | 3               | 6               | 7               | 0               | 18    | 0.2      | 0.73    | 0.14                | 0.15       |
| 13       | 0                    | 4               | 3               | 2               | 0               | 9     | 0.24     | 0.71    | 0.18                | 0.16       |
| 14       | 1                    | 3               | 2               | 4               | 0               | 10    | 0.23     | 0.73    | 0.19                | 0.15       |
| 15       | 0                    | 3               | 5               | 4               | 0               | 12    | 0.21     | 0.73    | 0.19                | 0.12       |
| 16       | 0                    | 1               | 7               | 3               | 0               | 11    | 0.22     | 0.71    | 0.17                | 0.16       |
| 17       | 0                    | 1               | 3               | 1               | 0               | 5     | 0.26     | 0.71    | 0.23                | 0.16       |
| 18       | 0                    | 3               | 3               | 1               | 0               | 7     | 0.29     | 0.7     | 0.21                | 0.2        |
| 19       | 2                    | 2               | 6               | 2               | 0               | 12    | 0.19     | 0.69    | 0.15                | 0.14       |
| 20       | 2                    | 4               | 4               | 1               | 0               | 11    | 0.18     | 0.35    | 0.09                | 0.13       |
| 21       | 0                    | 1               | 3               | 1               | 0               | 5     | 0.28     | 0.72    | 0.22                | 0.19       |
| 22       | 0                    | 4               | 3               | 5               | 0               | 12    | 0.22     | 0.72    | 0.17                | 0.16       |
| 23       | 1                    | 0               | 4               | 2               | 0               | 7     | 0.25     | 0.74    | 0.21                | 0.17       |
| 24       | 0                    | 1               | 7               | 1               | 0               | 9     | 0.22     | 0.73    | 0.18                | 0.14       |
| 25       | 1                    | 1               | 2               | 3               | 0               | 7     | 0.21     | 0.61    | 0.17                | 0.12       |
| 26       | 0                    | 1               | 3               | 0               | 0               | 4     | 0.3      | 0.71    | 0.24                | 0.19       |
| 27       | 0                    | 1               | 2               | 1               | 0               | 4     | 0.3      | 0.71    | 0.24                | 0.19       |
| 28       | 1                    | 6               | 6               | 9               | 0               | 22    | 0.19     | 0.73    | 0.14                | 0.15       |
| 29       | 0                    | 1               | 1               | 0               | 0               | 2     | 0.46     | 0.71    | 0.24                | 0.46       |
| 30       | 4                    | 3               | 3               | 2               | 0               | 12    | 0.18     | 0.44    | 0.09                | 0.15       |
| 31       | 1                    | 1               | 5               | 3               | 0               | 10    | 0.22     | 0.73    | 0.18                | 0.15       |
| 32       | 0                    | 2               | 5               | 2               | 0               | 9     | 0.22     | 0.72    | 0.18                | 0.16       |
| 33       | 0                    | 1               | 2               | 0               | 0               | 3     | 0.33     | 0.72    | 0.27                | 0.14       |
| 34       | 1                    | 1               | 2               | 0               | 0               | 4     | 0.32     | 0.71    | 0.23                | 0.23       |
| 35       | 0                    | 0               | 2               | 0               | 0               | 2     | 0.44     | 0.71    | 0.28                | 0.44       |
| 36       | 0                    | 0               | 4               | 0               | 0               | 4     | 0.26     | 0.68    | 0.24                | 0.13       |
| 37       | 0                    | 1               | 2               | 0               | 0               | 3     | 0.34     | 0.71    | 0.26                | 0.19       |
| 38       | 1                    | 1               | 3               | 2               | 0               | 7     | 0.21     | 0.7     | 0.2                 | 0.13       |
| 39       | 0                    | 1               | 3               | 0               | 0               | 4     | 0.28     | 0.71    | 0.25                | 0.16       |
| 40       | 1                    | 1               | 3               | 3               | 0               | 8     | 0.24     | 0.73    | 0.2                 | 0.15       |

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

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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 [i](#)

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, 2773(IR:827, SQ:847, MR:529, LR:570, 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>       | %    |
| 3                             | 5               | 9               | 7               | 0               | 24    | 1                        | 2.5  |
| 1                             | 4               | 5               | 5               | 0               | 15    | 2                        | 5.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 3                        | 7.5  |
| 0                             | 1               | 1               | 2               | 0               | 4     | 4                        | 10.0 |
| 0                             | 1               | 3               | 3               | 0               | 7     | 5                        | 12.5 |
| 0                             | 1               | 0               | 1               | 0               | 2     | 6                        | 15.0 |

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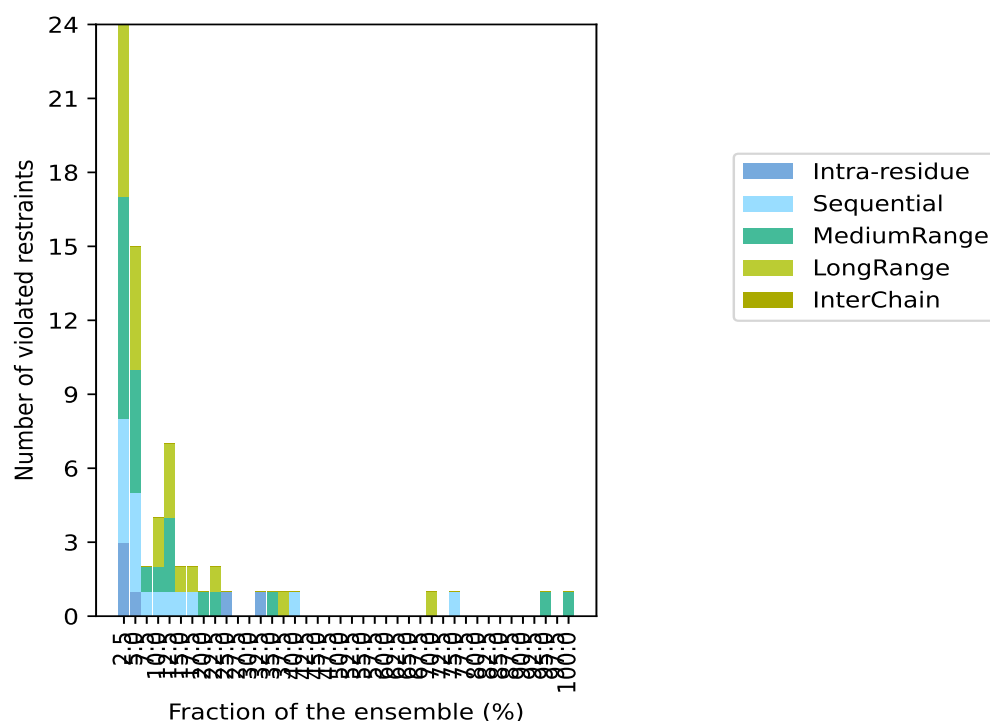
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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                             | 1               | 0               | 1               | 0               | 2     | 7                        | 17.5  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 8                        | 20.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 9                        | 22.5  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 10                       | 25.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 27.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 12                       | 30.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 13                       | 32.5  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 14                       | 35.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 15                       | 37.5  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 16                       | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 42.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 18                       | 45.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 19                       | 47.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 20                       | 50.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 21                       | 52.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 22                       | 55.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 23                       | 57.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 24                       | 60.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 25                       | 62.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 26                       | 65.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 27                       | 67.5  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 28                       | 70.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 29                       | 72.5  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 30                       | 75.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 31                       | 77.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 32                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 33                       | 82.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 34                       | 85.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 35                       | 87.5  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 36                       | 90.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 37                       | 92.5  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 38                       | 95.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 39                       | 97.5  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 40                       | 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

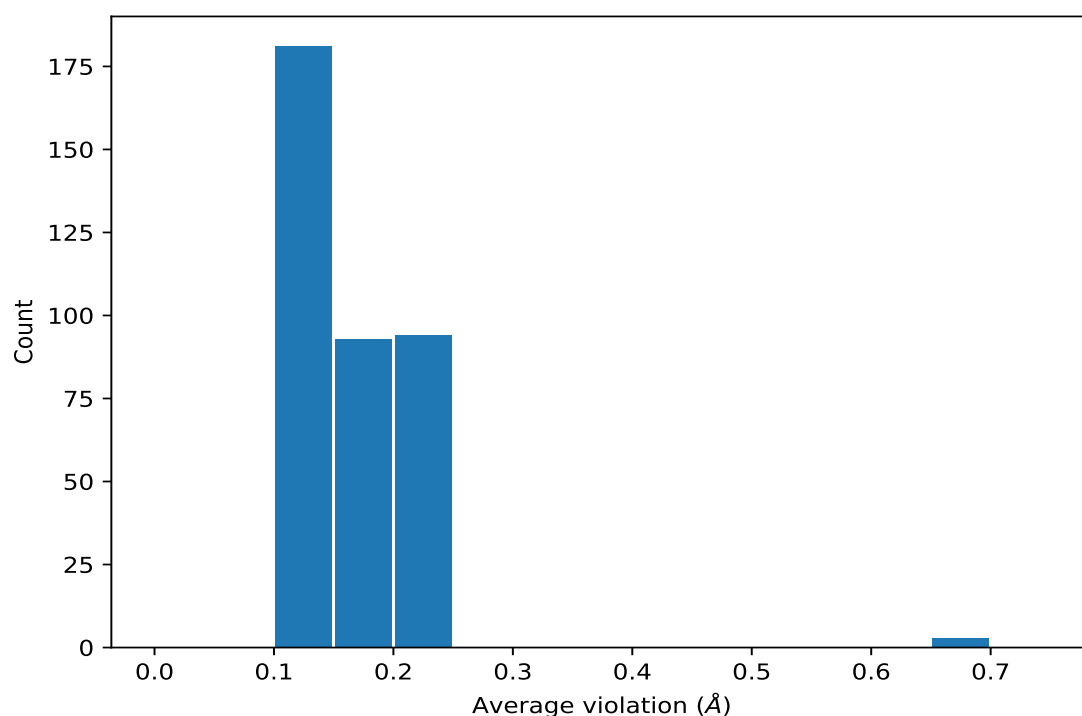
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1  | 40                  | 0.69     | 0.09                | 0.71       |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2  | 40                  | 0.69     | 0.09                | 0.71       |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3  | 40                  | 0.69     | 0.09                | 0.71       |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 38                  | 0.2      | 0.05                | 0.2        |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 30                  | 0.24     | 0.11                | 0.22       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 30                  | 0.24     | 0.11                | 0.22       |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 28                  | 0.15     | 0.04                | 0.14       |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 28                  | 0.15     | 0.04                | 0.14       |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 28                  | 0.15     | 0.04                | 0.14       |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 28                  | 0.15     | 0.04                | 0.14       |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 28                  | 0.15     | 0.04                | 0.14       |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 28                  | 0.15     | 0.04                | 0.14       |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 16                  | 0.13     | 0.02                | 0.12       |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 16                  | 0.13     | 0.02                | 0.12       |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 15                  | 0.15     | 0.03                | 0.14       |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 15                  | 0.15     | 0.03                | 0.14       |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 15                  | 0.15     | 0.03                | 0.14       |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 15                  | 0.15     | 0.03                | 0.14       |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 15                  | 0.15     | 0.03                | 0.14       |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 15                  | 0.15     | 0.03                | 0.14       |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 14                  | 0.21     | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 14                  | 0.21     | 0.08                | 0.18       |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 13                  | 0.13     | 0.03                | 0.13       |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 13                  | 0.13     | 0.03                | 0.13       |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 13                  | 0.13     | 0.03                | 0.13       |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 10                  | 0.22     | 0.06                | 0.22       |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2  | 9                   | 0.17     | 0.04                | 0.18       |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H    | 9                   | 0.12     | 0.02                | 0.11       |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H    | 9                   | 0.12     | 0.02                | 0.11       |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H    | 9                   | 0.12     | 0.02                | 0.11       |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H    | 9                   | 0.12     | 0.02                | 0.11       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H    | 9                   | 0.12     | 0.02                | 0.11       |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H    | 9                   | 0.12     | 0.02                | 0.11       |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3  | 8                   | 0.15     | 0.06                | 0.12       |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG11 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG12 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG13 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG21 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG22 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG23 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG11 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG12 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG13 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG21 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG22 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG23 | 7                   | 0.14     | 0.02                | 0.14       |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD11 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD12 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD13 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD21 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD22 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD23 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD11 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD12 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD13 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD21 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD22 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD23 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD11 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD12 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD13 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD21 | 7                   | 0.12     | 0.01                | 0.12       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD22 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD23 | 7                   | 0.12     | 0.01                | 0.12       |
| (1,2536) | 1:411:A:VAL:HG11 | 1:412:A:ILE:HB   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,2536) | 1:411:A:VAL:HG12 | 1:412:A:ILE:HB   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,2536) | 1:411:A:VAL:HG13 | 1:412:A:ILE:HB   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,2536) | 1:411:A:VAL:HG21 | 1:412:A:ILE:HB   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,2536) | 1:411:A:VAL:HG22 | 1:412:A:ILE:HB   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,2536) | 1:411:A:VAL:HG23 | 1:412:A:ILE:HB   | 6                   | 0.12     | 0.01                | 0.12       |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG21 | 6                   | 0.11     | 0.01                | 0.1        |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG22 | 6                   | 0.11     | 0.01                | 0.1        |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG23 | 6                   | 0.11     | 0.01                | 0.1        |
| (1,1809) | 1:429:A:VAL:HG11 | 1:431:A:GLU:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,1809) | 1:429:A:VAL:HG12 | 1:431:A:GLU:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,1809) | 1:429:A:VAL:HG13 | 1:431:A:GLU:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,1809) | 1:429:A:VAL:HG21 | 1:431:A:GLU:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,1809) | 1:429:A:VAL:HG22 | 1:431:A:GLU:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,1809) | 1:429:A:VAL:HG23 | 1:431:A:GLU:H    | 5                   | 0.17     | 0.07                | 0.13       |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE1  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE2  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE3  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE1  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE2  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE3  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE1  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE2  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE3  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE1  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE2  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE3  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE1  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE2  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE3  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE1  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE2  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE3  | 5                   | 0.16     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD1  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD2  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD1  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD2  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD1  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD2  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD1  | 5                   | 0.15     | 0.04                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD2  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD1  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD2  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD1  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD2  | 5                   | 0.15     | 0.04                | 0.16       |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD11 | 5                   | 0.13     | 0.03                | 0.12       |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD12 | 5                   | 0.13     | 0.03                | 0.12       |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD13 | 5                   | 0.13     | 0.03                | 0.12       |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD21 | 5                   | 0.13     | 0.03                | 0.12       |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD22 | 5                   | 0.13     | 0.03                | 0.12       |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD23 | 5                   | 0.13     | 0.03                | 0.12       |
| (1,710)  | 1:436:A:ILE:HG21 | 1:438:A:GLN:HA   | 5                   | 0.13     | 0.01                | 0.12       |
| (1,710)  | 1:436:A:ILE:HG22 | 1:438:A:GLN:HA   | 5                   | 0.13     | 0.01                | 0.12       |
| (1,710)  | 1:436:A:ILE:HG23 | 1:438:A:GLN:HA   | 5                   | 0.13     | 0.01                | 0.12       |
| (1,610)  | 1:348:A:MET:HE1  | 1:352:A:LEU:HG   | 5                   | 0.11     | 0.02                | 0.1        |
| (1,610)  | 1:348:A:MET:HE2  | 1:352:A:LEU:HG   | 5                   | 0.11     | 0.02                | 0.1        |
| (1,610)  | 1:348:A:MET:HE3  | 1:352:A:LEU:HG   | 5                   | 0.11     | 0.02                | 0.1        |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD11 | 5                   | 0.11     | 0.02                | 0.11       |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD12 | 5                   | 0.11     | 0.02                | 0.11       |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD13 | 5                   | 0.11     | 0.02                | 0.11       |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD11 | 5                   | 0.11     | 0.02                | 0.11       |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD12 | 5                   | 0.11     | 0.02                | 0.11       |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD13 | 5                   | 0.11     | 0.02                | 0.11       |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA2  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA3  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA2  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA3  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA2  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA3  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA2  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA3  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA2  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA3  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA2  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA3  | 4                   | 0.23     | 0.04                | 0.22       |
| (1,1981) | 1:368:A:LEU:HD11 | 1:369:A:ASP:H    | 4                   | 0.16     | 0.02                | 0.15       |
| (1,1981) | 1:368:A:LEU:HD12 | 1:369:A:ASP:H    | 4                   | 0.16     | 0.02                | 0.15       |
| (1,1981) | 1:368:A:LEU:HD13 | 1:369:A:ASP:H    | 4                   | 0.16     | 0.02                | 0.15       |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG21 | 4                   | 0.15     | 0.03                | 0.14       |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG22 | 4                   | 0.15     | 0.03                | 0.14       |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG23 | 4                   | 0.15     | 0.03                | 0.14       |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG21 | 4                   | 0.15     | 0.03                | 0.14       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG22 | 4                   | 0.15     | 0.03                | 0.14       |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG23 | 4                   | 0.15     | 0.03                | 0.14       |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG11 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG12 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG13 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG23 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG11 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG12 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG13 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG23 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG11 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG12 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG13 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG21 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG22 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG23 | 4                   | 0.13     | 0.02                | 0.12       |
| (1,2794) | 1:526:A:LEU:HD11 | 1:530:A:GLU:HB2  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD11 | 1:530:A:GLU:HB3  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD12 | 1:530:A:GLU:HB2  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD12 | 1:530:A:GLU:HB3  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD13 | 1:530:A:GLU:HB2  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD13 | 1:530:A:GLU:HB3  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD21 | 1:530:A:GLU:HB2  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD21 | 1:530:A:GLU:HB3  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD22 | 1:530:A:GLU:HB2  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD22 | 1:530:A:GLU:HB3  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD23 | 1:530:A:GLU:HB2  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2794) | 1:526:A:LEU:HD23 | 1:530:A:GLU:HB3  | 3                   | 0.23     | 0.04                | 0.23       |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD11 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD12 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD13 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD21 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD22 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD23 | 3                   | 0.14     | 0.02                | 0.16       |
| (1,1816) | 1:429:A:VAL:HG11 | 1:430:A:GLY:H    | 2                   | 0.2      | 0.04                | 0.2        |
| (1,1816) | 1:429:A:VAL:HG12 | 1:430:A:GLY:H    | 2                   | 0.2      | 0.04                | 0.2        |
| (1,1816) | 1:429:A:VAL:HG13 | 1:430:A:GLY:H    | 2                   | 0.2      | 0.04                | 0.2        |
| (1,1816) | 1:429:A:VAL:HG21 | 1:430:A:GLY:H    | 2                   | 0.2      | 0.04                | 0.2        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1816) | 1:429:A:VAL:HG22 | 1:430:A:GLY:H    | 2                   | 0.2      | 0.04                | 0.2        |
| (1,1816) | 1:429:A:VAL:HG23 | 1:430:A:GLY:H    | 2                   | 0.2      | 0.04                | 0.2        |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD11 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD12 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD13 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD21 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD22 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD23 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD11 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD12 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD13 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD21 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD22 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD23 | 2                   | 0.18     | 0.04                | 0.18       |
| (1,2114) | 1:352:A:LEU:HD11 | 1:393:A:HIS:HD2  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,2114) | 1:352:A:LEU:HD12 | 1:393:A:HIS:HD2  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,2114) | 1:352:A:LEU:HD13 | 1:393:A:HIS:HD2  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,2114) | 1:352:A:LEU:HD21 | 1:393:A:HIS:HD2  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,2114) | 1:352:A:LEU:HD22 | 1:393:A:HIS:HD2  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,2114) | 1:352:A:LEU:HD23 | 1:393:A:HIS:HD2  | 2                   | 0.18     | 0.05                | 0.18       |
| (1,1757) | 1:505:A:VAL:HG11 | 1:507:A:GLU:H    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1757) | 1:505:A:VAL:HG12 | 1:507:A:GLU:H    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1757) | 1:505:A:VAL:HG13 | 1:507:A:GLU:H    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1757) | 1:505:A:VAL:HG21 | 1:507:A:GLU:H    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1757) | 1:505:A:VAL:HG22 | 1:507:A:GLU:H    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1757) | 1:505:A:VAL:HG23 | 1:507:A:GLU:H    | 2                   | 0.18     | 0.03                | 0.18       |
| (1,1808) | 1:429:A:VAL:HG11 | 1:432:A:GLY:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1808) | 1:429:A:VAL:HG12 | 1:432:A:GLY:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1808) | 1:429:A:VAL:HG13 | 1:432:A:GLY:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1808) | 1:429:A:VAL:HG21 | 1:432:A:GLY:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1808) | 1:429:A:VAL:HG22 | 1:432:A:GLY:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,1808) | 1:429:A:VAL:HG23 | 1:432:A:GLY:H    | 2                   | 0.18     | 0.06                | 0.18       |
| (1,2632) | 1:440:A:LEU:HD11 | 1:441:A:ASN:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD11 | 1:441:A:ASN:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD12 | 1:441:A:ASN:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD12 | 1:441:A:ASN:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD13 | 1:441:A:ASN:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD13 | 1:441:A:ASN:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD21 | 1:441:A:ASN:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD21 | 1:441:A:ASN:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD22 | 1:441:A:ASN:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD22 | 1:441:A:ASN:HB3  | 2                   | 0.16     | 0.02                | 0.16       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2632) | 1:440:A:LEU:HD23 | 1:441:A:ASN:HB2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2632) | 1:440:A:LEU:HD23 | 1:441:A:ASN:HB3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2101) | 1:352:A:LEU:HD11 | 1:380:A:LEU:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2101) | 1:352:A:LEU:HD12 | 1:380:A:LEU:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2101) | 1:352:A:LEU:HD13 | 1:380:A:LEU:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2101) | 1:352:A:LEU:HD21 | 1:380:A:LEU:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2101) | 1:352:A:LEU:HD22 | 1:380:A:LEU:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2101) | 1:352:A:LEU:HD23 | 1:380:A:LEU:H    | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2073) | 1:348:A:MET:HE1  | 1:351:A:ARG:HD2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2073) | 1:348:A:MET:HE1  | 1:351:A:ARG:HD3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2073) | 1:348:A:MET:HE2  | 1:351:A:ARG:HD2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2073) | 1:348:A:MET:HE2  | 1:351:A:ARG:HD3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2073) | 1:348:A:MET:HE3  | 1:351:A:ARG:HD2  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2073) | 1:348:A:MET:HE3  | 1:351:A:ARG:HD3  | 2                   | 0.16     | 0.02                | 0.16       |
| (1,2621) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HB2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2621) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2621) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HB2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2621) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2621) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HB2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2621) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HB3  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD11 | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD12 | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD13 | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD21 | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD22 | 2                   | 0.15     | 0.03                | 0.15       |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD23 | 2                   | 0.15     | 0.03                | 0.15       |
| (1,38)   | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG11 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,38)   | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG12 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,38)   | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG13 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,38)   | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG11 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,38)   | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG12 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,38)   | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG13 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,38)   | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG11 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,38)   | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG12 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,38)   | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG13 | 2                   | 0.14     | 0.0                 | 0.14       |
| (1,2658) | 1:458:A:LEU:HB2  | 1:459:A:PHE:H    | 2                   | 0.13     | 0.02                | 0.13       |
| (1,2658) | 1:458:A:LEU:HB3  | 1:459:A:PHE:H    | 2                   | 0.13     | 0.02                | 0.13       |
| (1,342)  | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG11 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,342)  | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG12 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,342)  | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG13 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,342)  | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG11 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,342)  | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG12 | 2                   | 0.11     | 0.01                | 0.11       |

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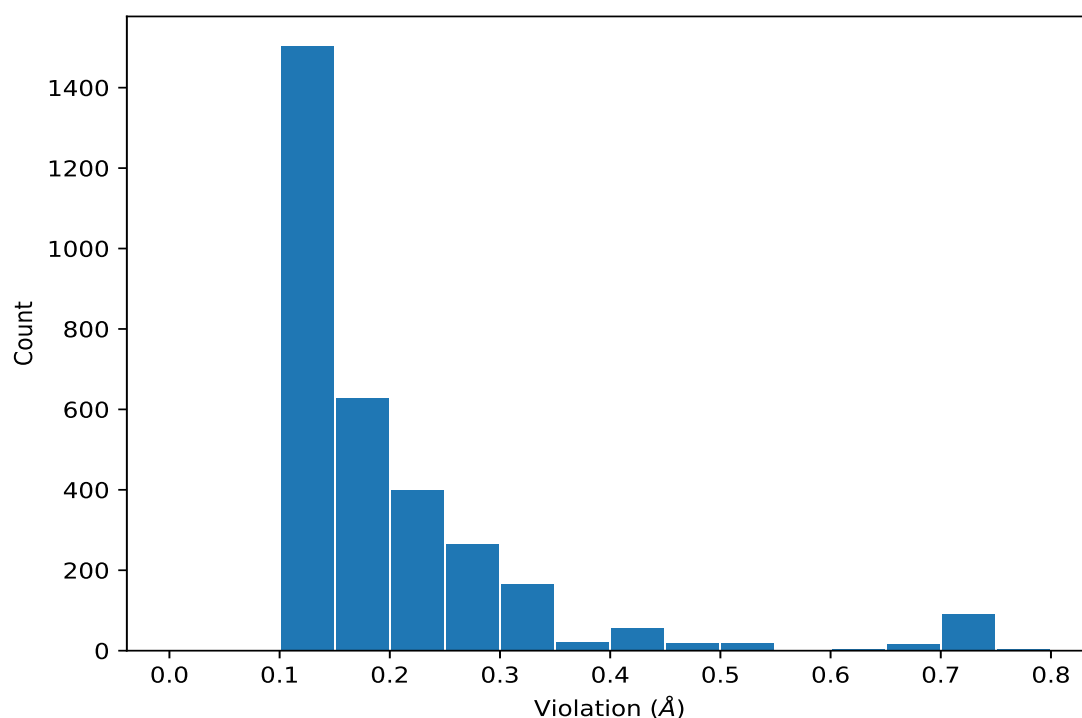
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,342)  | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG13 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,342)  | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG11 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,342)  | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG12 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,342)  | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG13 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE1  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2221) | 1:365:A:ILE:HG21 | 1:492:A:ASN:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2221) | 1:365:A:ILE:HG21 | 1:492:A:ASN:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2221) | 1:365:A:ILE:HG22 | 1:492:A:ASN:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2221) | 1:365:A:ILE:HG22 | 1:492:A:ASN:HD22 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2221) | 1:365:A:ILE:HG23 | 1:492:A:ASN:HD21 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,2221) | 1:365:A:ILE:HG23 | 1:492:A:ASN:HD22 | 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 ⓘ

### 9.5.1 Histogram : Distribution of distance violations ⓘ

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) |
|---------|------------------|-----------------|----------|---------------|
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 3        | 0.76          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 3        | 0.76          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 3        | 0.76          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 23       | 0.74          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 23       | 0.74          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 23       | 0.74          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 4        | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 4        | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 4        | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 11       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 11       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 11       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 12       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 12       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 12       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 14       | 0.73          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 14       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 14       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 15       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 15       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 15       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 24       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 24       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 24       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 28       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 28       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 28       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 31       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 31       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 31       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 40       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 40       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 40       | 0.73          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 6        | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 6        | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 6        | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 9        | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 9        | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 9        | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 21       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 21       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 21       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 22       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 22       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 22       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 32       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 32       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 32       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 33       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 33       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 33       | 0.72          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 2        | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 2        | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 2        | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 5        | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 5        | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 5        | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 8        | 0.71          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 8        | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 8        | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 10       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 10       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 10       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 13       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 13       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 13       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 16       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 16       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 16       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 17       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 17       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 17       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 26       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 26       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 26       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 27       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 27       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 27       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 29       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 29       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 29       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 34       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 34       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 34       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 35       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 35       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 35       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 37       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 37       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 37       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 39       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 39       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 39       | 0.71          |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 7        | 0.7           |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 7        | 0.7           |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 7        | 0.7           |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 18       | 0.7           |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 18       | 0.7           |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 18       | 0.7           |
| (1,798) | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 38       | 0.7           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 38       | 0.7           |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 38       | 0.7           |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 19       | 0.69          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 19       | 0.69          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 19       | 0.69          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 36       | 0.68          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 36       | 0.68          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 36       | 0.68          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 25       | 0.61          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 25       | 0.61          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 25       | 0.61          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 18       | 0.5           |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 15       | 0.46          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 15       | 0.46          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 28       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 28       | 0.44          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 30       | 0.44          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 30       | 0.44          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 30       | 0.44          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 14       | 0.42          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 14       | 0.42          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 11       | 0.4           |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 22       | 0.38          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 22       | 0.38          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 1        | 0.36          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2 | 1        | 0.36          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3 | 1        | 0.36          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB1 | 20       | 0.35          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB2  | 20       | 0.35          |
| (1,798)  | 1:471:A:ASN:HD21 | 1:474:A:ALA:HB3  | 20       | 0.35          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 6        | 0.34          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 6        | 0.34          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 16       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 16       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 23       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 23       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 23       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 13       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 20       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 20       | 0.33          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 20       | 0.33          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 9        | 0.32          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 9        | 0.32          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 20       | 0.31          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 30       | 0.3           |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA2  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA3  | 40       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA2  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA3  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA2  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA3  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA2  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA3  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA2  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA3  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA2  | 40       | 0.29          |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA3  | 40       | 0.29          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2  | 5        | 0.29          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3  | 5        | 0.29          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 31       | 0.29          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 31       | 0.29          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 31       | 0.29          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 2        | 0.29          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 2        | 0.29          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 2        | 0.29          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 2        | 0.29          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 2        | 0.29          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 2        | 0.29          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 2        | 0.29          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 2        | 0.29          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 2        | 0.29          |
| (1,2794) | 1:526:A:LEU:HD11 | 1:530:A:GLU:HB2  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD11 | 1:530:A:GLU:HB3  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD12 | 1:530:A:GLU:HB2  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD12 | 1:530:A:GLU:HB3  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD13 | 1:530:A:GLU:HB2  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD13 | 1:530:A:GLU:HB3  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD21 | 1:530:A:GLU:HB2  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD21 | 1:530:A:GLU:HB3  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD22 | 1:530:A:GLU:HB2  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD22 | 1:530:A:GLU:HB3  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD23 | 1:530:A:GLU:HB2  | 12       | 0.28          |
| (1,2794) | 1:526:A:LEU:HD23 | 1:530:A:GLU:HB3  | 12       | 0.28          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 3        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 3        | 0.28          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 3        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 5        | 0.28          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 5        | 0.28          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 3        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 5        | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 12       | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 12       | 0.28          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 12       | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 12       | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 12       | 0.28          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 12       | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 12       | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 12       | 0.28          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 12       | 0.28          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 1        | 0.27          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 12       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 12       | 0.26          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 12       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 26       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 26       | 0.26          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 26       | 0.26          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 6        | 0.26          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 6        | 0.26          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 6        | 0.26          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 6        | 0.26          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 6        | 0.26          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 6        | 0.26          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 6        | 0.26          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 6        | 0.26          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 6        | 0.26          |
| (1,1809) | 1:429:A:VAL:HG11 | 1:431:A:GLU:H    | 5        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG12 | 1:431:A:GLU:H    | 5        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG13 | 1:431:A:GLU:H    | 5        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG21 | 1:431:A:GLU:H    | 5        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG22 | 1:431:A:GLU:H    | 5        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG23 | 1:431:A:GLU:H    | 5        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG11 | 1:431:A:GLU:H    | 9        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG12 | 1:431:A:GLU:H    | 9        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG13 | 1:431:A:GLU:H    | 9        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG21 | 1:431:A:GLU:H    | 9        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG22 | 1:431:A:GLU:H    | 9        | 0.25          |
| (1,1809) | 1:429:A:VAL:HG23 | 1:431:A:GLU:H    | 9        | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 16       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 31       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 31       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 31       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 31       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 31       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 31       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 31       | 0.25          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 31       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 31       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 40       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 40       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 40       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 40       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 40       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 40       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 40       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 40       | 0.25          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 40       | 0.25          |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA2  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA3  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA2  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA3  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA2  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA3  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA2  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA3  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA2  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA3  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA2  | 21       | 0.24          |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA3  | 21       | 0.24          |
| (1,2114) | 1:352:A:LEU:HD11 | 1:393:A:HIS:HD2  | 4        | 0.24          |
| (1,2114) | 1:352:A:LEU:HD12 | 1:393:A:HIS:HD2  | 4        | 0.24          |
| (1,2114) | 1:352:A:LEU:HD13 | 1:393:A:HIS:HD2  | 4        | 0.24          |
| (1,2114) | 1:352:A:LEU:HD21 | 1:393:A:HIS:HD2  | 4        | 0.24          |
| (1,2114) | 1:352:A:LEU:HD22 | 1:393:A:HIS:HD2  | 4        | 0.24          |
| (1,2114) | 1:352:A:LEU:HD23 | 1:393:A:HIS:HD2  | 4        | 0.24          |
| (1,1816) | 1:429:A:VAL:HG11 | 1:430:A:GLY:H    | 32       | 0.24          |
| (1,1816) | 1:429:A:VAL:HG12 | 1:430:A:GLY:H    | 32       | 0.24          |
| (1,1816) | 1:429:A:VAL:HG13 | 1:430:A:GLY:H    | 32       | 0.24          |
| (1,1816) | 1:429:A:VAL:HG21 | 1:430:A:GLY:H    | 32       | 0.24          |
| (1,1816) | 1:429:A:VAL:HG22 | 1:430:A:GLY:H    | 32       | 0.24          |
| (1,1816) | 1:429:A:VAL:HG23 | 1:430:A:GLY:H    | 32       | 0.24          |
| (1,1808) | 1:429:A:VAL:HG11 | 1:432:A:GLY:H    | 22       | 0.24          |
| (1,1808) | 1:429:A:VAL:HG12 | 1:432:A:GLY:H    | 22       | 0.24          |
| (1,1808) | 1:429:A:VAL:HG13 | 1:432:A:GLY:H    | 22       | 0.24          |
| (1,1808) | 1:429:A:VAL:HG21 | 1:432:A:GLY:H    | 22       | 0.24          |
| (1,1808) | 1:429:A:VAL:HG22 | 1:432:A:GLY:H    | 22       | 0.24          |
| (1,1808) | 1:429:A:VAL:HG23 | 1:432:A:GLY:H    | 22       | 0.24          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 34       | 0.24          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 10       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 15       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 15       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 15       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 15       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 15       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 15       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 15       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 15       | 0.24          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 15       | 0.24          |
| (1,2794) | 1:526:A:LEU:HD11 | 1:530:A:GLU:HB2  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD11 | 1:530:A:GLU:HB3  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD12 | 1:530:A:GLU:HB2  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD12 | 1:530:A:GLU:HB3  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD13 | 1:530:A:GLU:HB2  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD13 | 1:530:A:GLU:HB3  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD21 | 1:530:A:GLU:HB2  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD21 | 1:530:A:GLU:HB3  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD22 | 1:530:A:GLU:HB2  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD22 | 1:530:A:GLU:HB3  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD23 | 1:530:A:GLU:HB2  | 3        | 0.23          |
| (1,2794) | 1:526:A:LEU:HD23 | 1:530:A:GLU:HB3  | 3        | 0.23          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 12       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 12       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 27       | 0.23          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 27       | 0.23          |
| (1,1619) | 1:435:A:VAL:HG11 | 1:436:A:ILE:H    | 10       | 0.23          |
| (1,1619) | 1:435:A:VAL:HG12 | 1:436:A:ILE:H    | 10       | 0.23          |
| (1,1619) | 1:435:A:VAL:HG13 | 1:436:A:ILE:H    | 10       | 0.23          |
| (1,1619) | 1:435:A:VAL:HG21 | 1:436:A:ILE:H    | 10       | 0.23          |
| (1,1619) | 1:435:A:VAL:HG22 | 1:436:A:ILE:H    | 10       | 0.23          |
| (1,1619) | 1:435:A:VAL:HG23 | 1:436:A:ILE:H    | 10       | 0.23          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 25       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 28       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 28       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 28       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 28       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 28       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 28       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 28       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 28       | 0.23          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 28       | 0.23          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1  | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2  | 10       | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2 | 10       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1 | 24       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2 | 24       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 29       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 34       | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 34       | 0.22          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 34       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE1  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE2  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE3  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE1  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE2  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE3  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE1  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE2  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE3  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE1  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE2  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE3  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE1  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE2  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE3  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE1  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE2  | 31       | 0.22          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE3  | 31       | 0.22          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD11 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD12 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD13 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD21 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD22 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD23 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD11 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD12 | 2        | 0.22          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD13 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD21 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD22 | 2        | 0.22          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD23 | 2        | 0.22          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 19       | 0.22          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 28       | 0.22          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 2        | 0.22          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 2        | 0.22          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 2        | 0.22          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 2        | 0.22          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 2        | 0.22          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 2        | 0.22          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 16       | 0.22          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 16       | 0.22          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 16       | 0.22          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 16       | 0.22          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 16       | 0.22          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 16       | 0.22          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2  | 1        | 0.21          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1  | 16       | 0.21          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2  | 16       | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA2  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA3  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA2  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA3  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA2  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA3  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA2  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA3  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA2  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA3  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA2  | 24       | 0.21          |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA3  | 24       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 17       | 0.21          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 17       | 0.21          |
| (1,1757) | 1:505:A:VAL:HG11 | 1:507:A:GLU:H    | 3        | 0.21          |
| (1,1757) | 1:505:A:VAL:HG12 | 1:507:A:GLU:H    | 3        | 0.21          |
| (1,1757) | 1:505:A:VAL:HG13 | 1:507:A:GLU:H    | 3        | 0.21          |
| (1,1757) | 1:505:A:VAL:HG21 | 1:507:A:GLU:H    | 3        | 0.21          |
| (1,1757) | 1:505:A:VAL:HG22 | 1:507:A:GLU:H    | 3        | 0.21          |
| (1,1757) | 1:505:A:VAL:HG23 | 1:507:A:GLU:H    | 3        | 0.21          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 7        | 0.21          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 8        | 0.21          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 8        | 0.21          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 8        | 0.21          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 8        | 0.21          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 8        | 0.21          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 8        | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 8        | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 8        | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 8        | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 13       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 14       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 20       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 22       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 22       | 0.21          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 22       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 22       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 22       | 0.21          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 22       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 22       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 22       | 0.21          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 22       | 0.21          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 3        | 0.21          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 3        | 0.21          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 3        | 0.21          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 3        | 0.21          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 3        | 0.21          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 3        | 0.21          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 10       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 10       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 10       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 10       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 10       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 10       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 12       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 12       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 12       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 12       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 12       | 0.21          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 12       | 0.21          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 9        | 0.21          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 9        | 0.21          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 9        | 0.21          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 9        | 0.21          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 9        | 0.21          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 9        | 0.21          |
| (1,1981) | 1:368:A:LEU:HD11 | 1:369:A:ASP:H    | 28       | 0.2           |
| (1,1981) | 1:368:A:LEU:HD12 | 1:369:A:ASP:H    | 28       | 0.2           |
| (1,1981) | 1:368:A:LEU:HD13 | 1:369:A:ASP:H    | 28       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 4        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 9        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 9        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 9        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 9        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 9        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 9        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 9        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 9        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 9        | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 11       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 18       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 18       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 18       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 18       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 18       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 18       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 18       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 18       | 0.2           |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 18       | 0.2           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 5        | 0.2           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 5        | 0.2           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 5        | 0.2           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 5        | 0.2           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 5        | 0.2           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 5        | 0.2           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 18       | 0.2           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 18       | 0.2           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 18       | 0.2           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 18       | 0.2           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 18       | 0.2           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 18       | 0.2           |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 5        | 0.19          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 5        | 0.19          |
| (1,2632) | 1:440:A:LEU:HD11 | 1:441:A:ASN:HB2  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD11 | 1:441:A:ASN:HB3  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD12 | 1:441:A:ASN:HB2  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD12 | 1:441:A:ASN:HB3  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD13 | 1:441:A:ASN:HB2  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD13 | 1:441:A:ASN:HB3  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD21 | 1:441:A:ASN:HB2  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD21 | 1:441:A:ASN:HB3  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD22 | 1:441:A:ASN:HB2  | 13       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2632) | 1:440:A:LEU:HD22 | 1:441:A:ASN:HB3  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD23 | 1:441:A:ASN:HB2  | 13       | 0.19          |
| (1,2632) | 1:440:A:LEU:HD23 | 1:441:A:ASN:HB3  | 13       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 39       | 0.19          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 39       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 21       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 21       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 37       | 0.19          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 37       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD1 | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD2 | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD1 | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD2 | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD1 | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD2 | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD1 | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD2 | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD1 | 10       | 0.19          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD2  | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD1  | 10       | 0.19          |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD2  | 10       | 0.19          |
| (1,2119) | 1:353:A:GLN:H    | 1:354:A:ARG:HG2  | 5        | 0.19          |
| (1,2119) | 1:353:A:GLN:H    | 1:354:A:ARG:HG3  | 5        | 0.19          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 30       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 32       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 32       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 32       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 32       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 32       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 32       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 32       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 32       | 0.19          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 32       | 0.19          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 6        | 0.19          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 6        | 0.19          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 6        | 0.19          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 6        | 0.19          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 6        | 0.19          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 6        | 0.19          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 10       | 0.19          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 10       | 0.19          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 10       | 0.19          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG21 | 5        | 0.19          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG22 | 5        | 0.19          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG23 | 5        | 0.19          |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG21 | 5        | 0.19          |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG22 | 5        | 0.19          |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG23 | 5        | 0.19          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 22       | 0.19          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 22       | 0.19          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 22       | 0.19          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 22       | 0.19          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1 | 22       | 0.19          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2 | 22       | 0.19          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1 | 6        | 0.18          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2 | 6        | 0.18          |
| (1,2621) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HB2 | 23       | 0.18          |
| (1,2621) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HB3 | 23       | 0.18          |
| (1,2621) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HB2 | 23       | 0.18          |
| (1,2621) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HB3 | 23       | 0.18          |
| (1,2621) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HB2 | 23       | 0.18          |
| (1,2621) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HB3 | 23       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA2 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG11 | 1:432:A:GLY:HA3 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA2 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG12 | 1:432:A:GLY:HA3 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA2 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG13 | 1:432:A:GLY:HA3 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA2 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG21 | 1:432:A:GLY:HA3 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA2 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG22 | 1:432:A:GLY:HA3 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA2 | 19       | 0.18          |
| (1,2613) | 1:429:A:VAL:HG23 | 1:432:A:GLY:HA3 | 19       | 0.18          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2 | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3 | 9        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2  | 9        | 0.18          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3  | 9        | 0.18          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 32       | 0.18          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 32       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD1  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD2  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD1  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD2  | 12       | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD1  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD2  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD1  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD2  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD1  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD2  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD1  | 12       | 0.18          |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD2  | 12       | 0.18          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD11 | 28       | 0.18          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD12 | 28       | 0.18          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD13 | 28       | 0.18          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD21 | 28       | 0.18          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD22 | 28       | 0.18          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD23 | 28       | 0.18          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE1  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE2  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE3  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE1  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE2  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE3  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE1  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE2  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE3  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE1  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE2  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE3  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE1  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE2  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE3  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE1  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE2  | 1        | 0.18          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE3  | 1        | 0.18          |
| (1,2101) | 1:352:A:LEU:HD11 | 1:380:A:LEU:H    | 10       | 0.18          |
| (1,2101) | 1:352:A:LEU:HD12 | 1:380:A:LEU:H    | 10       | 0.18          |
| (1,2101) | 1:352:A:LEU:HD13 | 1:380:A:LEU:H    | 10       | 0.18          |
| (1,2101) | 1:352:A:LEU:HD21 | 1:380:A:LEU:H    | 10       | 0.18          |
| (1,2101) | 1:352:A:LEU:HD22 | 1:380:A:LEU:H    | 10       | 0.18          |
| (1,2101) | 1:352:A:LEU:HD23 | 1:380:A:LEU:H    | 10       | 0.18          |
| (1,2073) | 1:348:A:MET:HE1  | 1:351:A:ARG:HD2  | 2        | 0.18          |
| (1,2073) | 1:348:A:MET:HE1  | 1:351:A:ARG:HD3  | 2        | 0.18          |
| (1,2073) | 1:348:A:MET:HE2  | 1:351:A:ARG:HD2  | 2        | 0.18          |
| (1,2073) | 1:348:A:MET:HE2  | 1:351:A:ARG:HD3  | 2        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2073) | 1:348:A:MET:HE3  | 1:351:A:ARG:HD2  | 2        | 0.18          |
| (1,2073) | 1:348:A:MET:HE3  | 1:351:A:ARG:HD3  | 2        | 0.18          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 25       | 0.18          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 25       | 0.18          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 25       | 0.18          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 25       | 0.18          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 25       | 0.18          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 25       | 0.18          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 25       | 0.18          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 25       | 0.18          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 25       | 0.18          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 12       | 0.18          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 12       | 0.18          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 12       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG21 | 1:476:A:ILE:HG21 | 28       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG21 | 1:476:A:ILE:HG22 | 28       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG21 | 1:476:A:ILE:HG23 | 28       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG22 | 1:476:A:ILE:HG21 | 28       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG22 | 1:476:A:ILE:HG22 | 28       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG22 | 1:476:A:ILE:HG23 | 28       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG23 | 1:476:A:ILE:HG21 | 28       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG23 | 1:476:A:ILE:HG22 | 28       | 0.18          |
| (1,472)  | 1:397:A:ILE:HG23 | 1:476:A:ILE:HG23 | 28       | 0.18          |
| (1,2794) | 1:526:A:LEU:HD11 | 1:530:A:GLU:HB2  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD11 | 1:530:A:GLU:HB3  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD12 | 1:530:A:GLU:HB2  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD12 | 1:530:A:GLU:HB3  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD13 | 1:530:A:GLU:HB2  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD13 | 1:530:A:GLU:HB3  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD21 | 1:530:A:GLU:HB2  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD21 | 1:530:A:GLU:HB3  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD22 | 1:530:A:GLU:HB2  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD22 | 1:530:A:GLU:HB3  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD23 | 1:530:A:GLU:HB2  | 7        | 0.17          |
| (1,2794) | 1:526:A:LEU:HD23 | 1:530:A:GLU:HB3  | 7        | 0.17          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD11 | 5        | 0.17          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD12 | 5        | 0.17          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD13 | 5        | 0.17          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD21 | 5        | 0.17          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD22 | 5        | 0.17          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD23 | 5        | 0.17          |
| (1,2386) | 1:386:A:THR:HG21 | 1:389:A:GLN:HE21 | 28       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2386) | 1:386:A:THR:HG21 | 1:389:A:GLN:HE22 | 28       | 0.17          |
| (1,2386) | 1:386:A:THR:HG22 | 1:389:A:GLN:HE21 | 28       | 0.17          |
| (1,2386) | 1:386:A:THR:HG22 | 1:389:A:GLN:HE22 | 28       | 0.17          |
| (1,2386) | 1:386:A:THR:HG23 | 1:389:A:GLN:HE21 | 28       | 0.17          |
| (1,2386) | 1:386:A:THR:HG23 | 1:389:A:GLN:HE22 | 28       | 0.17          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 4        | 0.17          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 4        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 8        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 8        | 0.17          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 8        | 0.17          |
| (1,999)  | 1:491:A:PHE:HD1  | 1:496:A:LEU:HD21 | 10       | 0.17          |
| (1,999)  | 1:491:A:PHE:HD1  | 1:496:A:LEU:HD22 | 10       | 0.17          |
| (1,999)  | 1:491:A:PHE:HD1  | 1:496:A:LEU:HD23 | 10       | 0.17          |
| (1,999)  | 1:491:A:PHE:HD2  | 1:496:A:LEU:HD21 | 10       | 0.17          |
| (1,999)  | 1:491:A:PHE:HD2  | 1:496:A:LEU:HD22 | 10       | 0.17          |
| (1,999)  | 1:491:A:PHE:HD2  | 1:496:A:LEU:HD23 | 10       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 1        | 0.17          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 23       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 24       | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 24       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 24       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 24       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 24       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 24       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 24       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 24       | 0.17          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 24       | 0.17          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 9        | 0.17          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 9        | 0.17          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 9        | 0.17          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 9        | 0.17          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 9        | 0.17          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 9        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 6        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 6        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 6        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 6        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 6        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 6        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 8        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 8        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 8        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 8        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 8        | 0.17          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 8        | 0.17          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1  | 13       | 0.16          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2  | 13       | 0.16          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 2        | 0.16          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 2        | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD11 | 18       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD12 | 18       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD13 | 18       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD21 | 18       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD22 | 18       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD23 | 18       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD11 | 30       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD12 | 30       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD13 | 30       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD21 | 30       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD22 | 30       | 0.16          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD23 | 30       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG11 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG12 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG13 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG21 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG22 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG23 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG11 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG12 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG13 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG21 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG22 | 28       | 0.16          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG23 | 28       | 0.16          |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H    | 10       | 0.16          |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H    | 10       | 0.16          |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H    | 10       | 0.16          |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H    | 10       | 0.16          |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H    | 10       | 0.16          |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H    | 10       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 16       | 0.16          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 16       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 30       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 32       | 0.16          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 32       | 0.16          |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD1 | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD2 | 2        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD1  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD2  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD1  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD2  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD1  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD2  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD1  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD2  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD1  | 2        | 0.16          |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD2  | 2        | 0.16          |
| (1,2172) | 1:361:A:ASN:HB2  | 1:364:A:LYS:HD2  | 28       | 0.16          |
| (1,2172) | 1:361:A:ASN:HB2  | 1:364:A:LYS:HD3  | 28       | 0.16          |
| (1,2172) | 1:361:A:ASN:HB3  | 1:364:A:LYS:HD2  | 28       | 0.16          |
| (1,2172) | 1:361:A:ASN:HB3  | 1:364:A:LYS:HD3  | 28       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE1  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE2  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE3  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE1  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE2  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE3  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE1  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE2  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE3  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE1  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE2  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE3  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE1  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE2  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE3  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE1  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE2  | 12       | 0.16          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE3  | 12       | 0.16          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG11 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG12 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG13 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG21 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG22 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG23 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG11 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG12 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG13 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG21 | 14       | 0.16          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2077) | 1:348:A:MET:HE2 | 1:385:A:VAL:HG22 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE2 | 1:385:A:VAL:HG23 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG11 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG12 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG13 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG21 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG22 | 14       | 0.16          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG23 | 14       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD11 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD12 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD13 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD11 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD12 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD13 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD11 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD12 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD13 | 7        | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD11 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD12 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD13 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD11 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD12 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD13 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD11 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD12 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD13 | 17       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD11 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD12 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD13 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD11 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD12 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD13 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD11 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD12 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD13 | 19       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD11 | 35       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD12 | 35       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB1 | 1:476:A:ILE:HD13 | 35       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD11 | 35       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD12 | 35       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB2 | 1:476:A:ILE:HD13 | 35       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3 | 1:476:A:ILE:HD11 | 35       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 35       | 0.16          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 35       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 11       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 11       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 11       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 11       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 11       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 11       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 22       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 22       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 22       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 22       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 22       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 22       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 30       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 30       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 30       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 30       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 30       | 0.16          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 30       | 0.16          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 3        | 0.16          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 3        | 0.16          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 3        | 0.16          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 40       | 0.16          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 40       | 0.16          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 40       | 0.16          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 40       | 0.16          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 40       | 0.16          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 40       | 0.16          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 19       | 0.15          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 19       | 0.15          |
| (1,2658) | 1:458:A:LEU:HB2  | 1:459:A:PHE:H    | 20       | 0.15          |
| (1,2658) | 1:458:A:LEU:HB3  | 1:459:A:PHE:H    | 20       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG11 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG12 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG13 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG21 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG22 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG23 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG11 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG12 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG13 | 6        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG21 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG22 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG23 | 6        | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG11 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG12 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG13 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG21 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG22 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG23 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG11 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG12 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG13 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG21 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG22 | 14       | 0.15          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG23 | 14       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 28       | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 28       | 0.15          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 28       | 0.15          |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H    | 3        | 0.15          |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H    | 3        | 0.15          |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H    | 3        | 0.15          |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H    | 3        | 0.15          |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H    | 3        | 0.15          |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H    | 3        | 0.15          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 10       | 0.15          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 10       | 0.15          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD11 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD12 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD13 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD21 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD22 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG2  | 1:352:A:LEU:HD23 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD11 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD12 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD13 | 6        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD21 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD22 | 6        | 0.15          |
| (1,2071) | 1:348:A:MET:HG3  | 1:352:A:LEU:HD23 | 6        | 0.15          |
| (1,1981) | 1:368:A:LEU:HD11 | 1:369:A:ASP:H    | 4        | 0.15          |
| (1,1981) | 1:368:A:LEU:HD12 | 1:369:A:ASP:H    | 4        | 0.15          |
| (1,1981) | 1:368:A:LEU:HD13 | 1:369:A:ASP:H    | 4        | 0.15          |
| (1,1981) | 1:368:A:LEU:HD11 | 1:369:A:ASP:H    | 8        | 0.15          |
| (1,1981) | 1:368:A:LEU:HD12 | 1:369:A:ASP:H    | 8        | 0.15          |
| (1,1981) | 1:368:A:LEU:HD13 | 1:369:A:ASP:H    | 8        | 0.15          |
| (1,1981) | 1:368:A:LEU:HD11 | 1:369:A:ASP:H    | 22       | 0.15          |
| (1,1981) | 1:368:A:LEU:HD12 | 1:369:A:ASP:H    | 22       | 0.15          |
| (1,1981) | 1:368:A:LEU:HD13 | 1:369:A:ASP:H    | 22       | 0.15          |
| (1,1816) | 1:429:A:VAL:HG11 | 1:430:A:GLY:H    | 13       | 0.15          |
| (1,1816) | 1:429:A:VAL:HG12 | 1:430:A:GLY:H    | 13       | 0.15          |
| (1,1816) | 1:429:A:VAL:HG13 | 1:430:A:GLY:H    | 13       | 0.15          |
| (1,1816) | 1:429:A:VAL:HG21 | 1:430:A:GLY:H    | 13       | 0.15          |
| (1,1816) | 1:429:A:VAL:HG22 | 1:430:A:GLY:H    | 13       | 0.15          |
| (1,1816) | 1:429:A:VAL:HG23 | 1:430:A:GLY:H    | 13       | 0.15          |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD11 | 2        | 0.15          |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD12 | 2        | 0.15          |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD13 | 2        | 0.15          |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD11 | 2        | 0.15          |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD12 | 2        | 0.15          |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD13 | 2        | 0.15          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 27       | 0.15          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 27       | 0.15          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 27       | 0.15          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 27       | 0.15          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 27       | 0.15          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 27       | 0.15          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 27       | 0.15          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 27       | 0.15          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 27       | 0.15          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 4        | 0.15          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 4        | 0.15          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 4        | 0.15          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 4        | 0.15          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 4        | 0.15          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 4        | 0.15          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 9        | 0.15          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 9        | 0.15          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 9        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 31       | 0.15          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 31       | 0.15          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 31       | 0.15          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 31       | 0.15          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 31       | 0.15          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 31       | 0.15          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 4        | 0.14          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 4        | 0.14          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 13       | 0.14          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 13       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD11 | 1:441:A:ASN:HB2  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD11 | 1:441:A:ASN:HB3  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD12 | 1:441:A:ASN:HB2  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD12 | 1:441:A:ASN:HB3  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD13 | 1:441:A:ASN:HB2  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD13 | 1:441:A:ASN:HB3  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD21 | 1:441:A:ASN:HB2  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD21 | 1:441:A:ASN:HB3  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD22 | 1:441:A:ASN:HB2  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD22 | 1:441:A:ASN:HB3  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD23 | 1:441:A:ASN:HB2  | 33       | 0.14          |
| (1,2632) | 1:440:A:LEU:HD23 | 1:441:A:ASN:HB3  | 33       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2  | 12       | 0.14          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3  | 12       | 0.14          |
| (1,2536) | 1:411:A:VAL:HG11 | 1:412:A:ILE:HB   | 10       | 0.14          |
| (1,2536) | 1:411:A:VAL:HG12 | 1:412:A:ILE:HB   | 10       | 0.14          |
| (1,2536) | 1:411:A:VAL:HG13 | 1:412:A:ILE:HB   | 10       | 0.14          |
| (1,2536) | 1:411:A:VAL:HG21 | 1:412:A:ILE:HB   | 10       | 0.14          |
| (1,2536) | 1:411:A:VAL:HG22 | 1:412:A:ILE:HB   | 10       | 0.14          |
| (1,2536) | 1:411:A:VAL:HG23 | 1:412:A:ILE:HB   | 10       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG11 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG12 | 31       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG13 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG21 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG22 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG23 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG11 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG12 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG13 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG21 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG22 | 31       | 0.14          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG23 | 31       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 36       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 36       | 0.14          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 36       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 1        | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 19       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 24       | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 24       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 40       | 0.14          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 40       | 0.14          |
| (1,2101) | 1:352:A:LEU:HD11 | 1:380:A:LEU:H   | 19       | 0.14          |
| (1,2101) | 1:352:A:LEU:HD12 | 1:380:A:LEU:H   | 19       | 0.14          |
| (1,2101) | 1:352:A:LEU:HD13 | 1:380:A:LEU:H   | 19       | 0.14          |
| (1,2101) | 1:352:A:LEU:HD21 | 1:380:A:LEU:H   | 19       | 0.14          |
| (1,2101) | 1:352:A:LEU:HD22 | 1:380:A:LEU:H   | 19       | 0.14          |
| (1,2101) | 1:352:A:LEU:HD23 | 1:380:A:LEU:H   | 19       | 0.14          |
| (1,1757) | 1:505:A:VAL:HG11 | 1:507:A:GLU:H   | 24       | 0.14          |
| (1,1757) | 1:505:A:VAL:HG12 | 1:507:A:GLU:H   | 24       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1757) | 1:505:A:VAL:HG13 | 1:507:A:GLU:H    | 24       | 0.14          |
| (1,1757) | 1:505:A:VAL:HG21 | 1:507:A:GLU:H    | 24       | 0.14          |
| (1,1757) | 1:505:A:VAL:HG22 | 1:507:A:GLU:H    | 24       | 0.14          |
| (1,1757) | 1:505:A:VAL:HG23 | 1:507:A:GLU:H    | 24       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 33       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 38       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 38       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 38       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 38       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 38       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 38       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 38       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 38       | 0.14          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 38       | 0.14          |
| (1,710)  | 1:436:A:ILE:HG21 | 1:438:A:GLN:HA   | 3        | 0.14          |
| (1,710)  | 1:436:A:ILE:HG22 | 1:438:A:GLN:HA   | 3        | 0.14          |
| (1,710)  | 1:436:A:ILE:HG23 | 1:438:A:GLN:HA   | 3        | 0.14          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 13       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 13       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 13       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 13       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 13       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 13       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 14       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 14       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 14       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 14       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 14       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 14       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 28       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 28       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 28       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 28       | 0.14          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 28       | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 28       | 0.14          |
| (1,610) | 1:348:A:MET:HE1  | 1:352:A:LEU:HG   | 9        | 0.14          |
| (1,610) | 1:348:A:MET:HE2  | 1:352:A:LEU:HG   | 9        | 0.14          |
| (1,610) | 1:348:A:MET:HE3  | 1:352:A:LEU:HG   | 9        | 0.14          |
| (1,585) | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG21 | 2        | 0.14          |
| (1,585) | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG22 | 2        | 0.14          |
| (1,585) | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG23 | 2        | 0.14          |
| (1,585) | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG21 | 2        | 0.14          |
| (1,585) | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG22 | 2        | 0.14          |
| (1,585) | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG23 | 2        | 0.14          |
| (1,117) | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 1        | 0.14          |
| (1,117) | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 1        | 0.14          |
| (1,117) | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 1        | 0.14          |
| (1,117) | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 1        | 0.14          |
| (1,117) | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 1        | 0.14          |
| (1,117) | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 1        | 0.14          |
| (1,117) | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 11       | 0.14          |
| (1,117) | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 11       | 0.14          |
| (1,117) | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 11       | 0.14          |
| (1,117) | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 11       | 0.14          |
| (1,117) | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 11       | 0.14          |
| (1,117) | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 11       | 0.14          |
| (1,117) | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 13       | 0.14          |
| (1,117) | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 13       | 0.14          |
| (1,117) | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 13       | 0.14          |
| (1,117) | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 13       | 0.14          |
| (1,117) | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 13       | 0.14          |
| (1,117) | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 13       | 0.14          |
| (1,117) | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 14       | 0.14          |
| (1,117) | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 14       | 0.14          |
| (1,117) | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 14       | 0.14          |
| (1,117) | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 14       | 0.14          |
| (1,117) | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 14       | 0.14          |
| (1,117) | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 14       | 0.14          |
| (1,38)  | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG11 | 22       | 0.14          |
| (1,38)  | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG12 | 22       | 0.14          |
| (1,38)  | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG13 | 22       | 0.14          |
| (1,38)  | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG11 | 22       | 0.14          |
| (1,38)  | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG12 | 22       | 0.14          |
| (1,38)  | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG13 | 22       | 0.14          |
| (1,38)  | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG11 | 22       | 0.14          |
| (1,38)  | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG12 | 22       | 0.14          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,38)   | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG13 | 22       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG11 | 28       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG12 | 28       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD11 | 1:385:A:VAL:HG13 | 28       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG11 | 28       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG12 | 28       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD12 | 1:385:A:VAL:HG13 | 28       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG11 | 28       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG12 | 28       | 0.14          |
| (1,38)   | 1:352:A:LEU:HD13 | 1:385:A:VAL:HG13 | 28       | 0.14          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1  | 19       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2  | 19       | 0.13          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 3        | 0.13          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 3        | 0.13          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 18       | 0.13          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 18       | 0.13          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 22       | 0.13          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 22       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG2  | 1:472:A:LEU:HD11 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG2  | 1:472:A:LEU:HD12 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG2  | 1:472:A:LEU:HD13 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG2  | 1:472:A:LEU:HD21 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG2  | 1:472:A:LEU:HD22 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG2  | 1:472:A:LEU:HD23 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG3  | 1:472:A:LEU:HD11 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG3  | 1:472:A:LEU:HD12 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG3  | 1:472:A:LEU:HD13 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG3  | 1:472:A:LEU:HD21 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG3  | 1:472:A:LEU:HD22 | 19       | 0.13          |
| (1,2672) | 1:468:A:GLU:HG3  | 1:472:A:LEU:HD23 | 19       | 0.13          |
| (1,2536) | 1:411:A:VAL:HG11 | 1:412:A:ILE:HB   | 3        | 0.13          |
| (1,2536) | 1:411:A:VAL:HG12 | 1:412:A:ILE:HB   | 3        | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2536) | 1:411:A:VAL:HG13 | 1:412:A:ILE:HB   | 3        | 0.13          |
| (1,2536) | 1:411:A:VAL:HG21 | 1:412:A:ILE:HB   | 3        | 0.13          |
| (1,2536) | 1:411:A:VAL:HG22 | 1:412:A:ILE:HB   | 3        | 0.13          |
| (1,2536) | 1:411:A:VAL:HG23 | 1:412:A:ILE:HB   | 3        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG11 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG12 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG13 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG21 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG22 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG23 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG11 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG12 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG13 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG21 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG22 | 1        | 0.13          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG23 | 1        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H    | 4        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H    | 4        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H    | 4        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H    | 4        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H    | 4        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H    | 4        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H    | 5        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H    | 5        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H    | 5        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H    | 5        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H    | 5        | 0.13          |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H    | 5        | 0.13          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD11 | 4        | 0.13          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD12 | 4        | 0.13          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD13 | 4        | 0.13          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD21 | 4        | 0.13          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD22 | 4        | 0.13          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD23 | 4        | 0.13          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE1  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE2  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE3  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE1  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE2  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE3  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE1  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE2  | 21       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE3  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE1  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE2  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE3  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE1  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE2  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE3  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE1  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE2  | 21       | 0.13          |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE3  | 21       | 0.13          |
| (1,2114) | 1:352:A:LEU:HD11 | 1:393:A:HIS:HD2  | 1        | 0.13          |
| (1,2114) | 1:352:A:LEU:HD12 | 1:393:A:HIS:HD2  | 1        | 0.13          |
| (1,2114) | 1:352:A:LEU:HD13 | 1:393:A:HIS:HD2  | 1        | 0.13          |
| (1,2114) | 1:352:A:LEU:HD21 | 1:393:A:HIS:HD2  | 1        | 0.13          |
| (1,2114) | 1:352:A:LEU:HD22 | 1:393:A:HIS:HD2  | 1        | 0.13          |
| (1,2114) | 1:352:A:LEU:HD23 | 1:393:A:HIS:HD2  | 1        | 0.13          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG11 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG12 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG13 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG21 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG22 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG23 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG11 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG12 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG13 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG21 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG22 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG23 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG11 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG12 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG13 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG21 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG22 | 38       | 0.13          |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG23 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD11 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD12 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD13 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD21 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD22 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD23 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD11 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD12 | 30       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD13 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD21 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD22 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD23 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD11 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD12 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD13 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD21 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD22 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD23 | 30       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD11 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD12 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD13 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD21 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD22 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD23 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD11 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD12 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD13 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD21 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD22 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD23 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD11 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD12 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD13 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD21 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD22 | 38       | 0.13          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD23 | 38       | 0.13          |
| (1,2073) | 1:348:A:MET:HE1  | 1:351:A:ARG:HD2  | 6        | 0.13          |
| (1,2073) | 1:348:A:MET:HE1  | 1:351:A:ARG:HD3  | 6        | 0.13          |
| (1,2073) | 1:348:A:MET:HE2  | 1:351:A:ARG:HD2  | 6        | 0.13          |
| (1,2073) | 1:348:A:MET:HE2  | 1:351:A:ARG:HD3  | 6        | 0.13          |
| (1,2073) | 1:348:A:MET:HE3  | 1:351:A:ARG:HD2  | 6        | 0.13          |
| (1,2073) | 1:348:A:MET:HE3  | 1:351:A:ARG:HD3  | 6        | 0.13          |
| (1,1809) | 1:429:A:VAL:HG11 | 1:431:A:GLU:H    | 32       | 0.13          |
| (1,1809) | 1:429:A:VAL:HG12 | 1:431:A:GLU:H    | 32       | 0.13          |
| (1,1809) | 1:429:A:VAL:HG13 | 1:431:A:GLU:H    | 32       | 0.13          |
| (1,1809) | 1:429:A:VAL:HG21 | 1:431:A:GLU:H    | 32       | 0.13          |
| (1,1809) | 1:429:A:VAL:HG22 | 1:431:A:GLU:H    | 32       | 0.13          |
| (1,1809) | 1:429:A:VAL:HG23 | 1:431:A:GLU:H    | 32       | 0.13          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 38       | 0.13          |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG21 | 15       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG22 | 15       | 0.13          |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG23 | 15       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 37       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 37       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 37       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 37       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 37       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 37       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 37       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 37       | 0.13          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 37       | 0.13          |
| (1,725)  | 1:436:A:ILE:HG21 | 1:438:A:GLN:HG2  | 16       | 0.13          |
| (1,725)  | 1:436:A:ILE:HG21 | 1:438:A:GLN:HG3  | 16       | 0.13          |
| (1,725)  | 1:436:A:ILE:HG22 | 1:438:A:GLN:HG2  | 16       | 0.13          |
| (1,725)  | 1:436:A:ILE:HG22 | 1:438:A:GLN:HG3  | 16       | 0.13          |
| (1,725)  | 1:436:A:ILE:HG23 | 1:438:A:GLN:HG2  | 16       | 0.13          |
| (1,725)  | 1:436:A:ILE:HG23 | 1:438:A:GLN:HG3  | 16       | 0.13          |
| (1,710)  | 1:436:A:ILE:HG21 | 1:438:A:GLN:HA   | 24       | 0.13          |
| (1,710)  | 1:436:A:ILE:HG22 | 1:438:A:GLN:HA   | 24       | 0.13          |
| (1,710)  | 1:436:A:ILE:HG23 | 1:438:A:GLN:HA   | 24       | 0.13          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 23       | 0.13          |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 23       | 0.13          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 23       | 0.13          |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 23       | 0.13          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 23       | 0.13          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 23       | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 8        | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 8        | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 8        | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 20       | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 20       | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 20       | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 30       | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 30       | 0.13          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 30       | 0.13          |
| (1,610)  | 1:348:A:MET:HE1  | 1:352:A:LEU:HG   | 12       | 0.13          |
| (1,610)  | 1:348:A:MET:HE2  | 1:352:A:LEU:HG   | 12       | 0.13          |
| (1,610)  | 1:348:A:MET:HE3  | 1:352:A:LEU:HG   | 12       | 0.13          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG21 | 10       | 0.13          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG22 | 10       | 0.13          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG23 | 10       | 0.13          |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG21 | 10       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG22 | 10       | 0.13          |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG23 | 10       | 0.13          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 4        | 0.13          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 4        | 0.13          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 4        | 0.13          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 4        | 0.13          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 4        | 0.13          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 4        | 0.13          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 23       | 0.13          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 23       | 0.13          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 23       | 0.13          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 23       | 0.13          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 23       | 0.13          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 23       | 0.13          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1  | 36       | 0.12          |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2  | 36       | 0.12          |
| (1,2772) | 1:518:A:LYS:H    | 1:518:A:LYS:HB2  | 30       | 0.12          |
| (1,2772) | 1:518:A:LYS:H    | 1:518:A:LYS:HB3  | 30       | 0.12          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 6        | 0.12          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 6        | 0.12          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 8        | 0.12          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 8        | 0.12          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 10       | 0.12          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 10       | 0.12          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 12       | 0.12          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 12       | 0.12          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD11 | 30       | 0.12          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD12 | 30       | 0.12          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD13 | 30       | 0.12          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD21 | 30       | 0.12          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD22 | 30       | 0.12          |
| (1,2656) | 1:458:A:LEU:HA   | 1:458:A:LEU:HD23 | 30       | 0.12          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2621) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HB2 | 32       | 0.12          |
| (1,2621) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HB3 | 32       | 0.12          |
| (1,2621) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HB2 | 32       | 0.12          |
| (1,2621) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HB3 | 32       | 0.12          |
| (1,2621) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HB2 | 32       | 0.12          |
| (1,2621) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HB3 | 32       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3 | 19       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3 | 24       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2 | 30       | 0.12          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3 | 30       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2536) | 1:411:A:VAL:HG11 | 1:412:A:ILE:HB   | 2        | 0.12          |
| (1,2536) | 1:411:A:VAL:HG12 | 1:412:A:ILE:HB   | 2        | 0.12          |
| (1,2536) | 1:411:A:VAL:HG13 | 1:412:A:ILE:HB   | 2        | 0.12          |
| (1,2536) | 1:411:A:VAL:HG21 | 1:412:A:ILE:HB   | 2        | 0.12          |
| (1,2536) | 1:411:A:VAL:HG22 | 1:412:A:ILE:HB   | 2        | 0.12          |
| (1,2536) | 1:411:A:VAL:HG23 | 1:412:A:ILE:HB   | 2        | 0.12          |
| (1,2536) | 1:411:A:VAL:HG11 | 1:412:A:ILE:HB   | 28       | 0.12          |
| (1,2536) | 1:411:A:VAL:HG12 | 1:412:A:ILE:HB   | 28       | 0.12          |
| (1,2536) | 1:411:A:VAL:HG13 | 1:412:A:ILE:HB   | 28       | 0.12          |
| (1,2536) | 1:411:A:VAL:HG21 | 1:412:A:ILE:HB   | 28       | 0.12          |
| (1,2536) | 1:411:A:VAL:HG22 | 1:412:A:ILE:HB   | 28       | 0.12          |
| (1,2536) | 1:411:A:VAL:HG23 | 1:412:A:ILE:HB   | 28       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG11 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG12 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG13 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG21 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG22 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG23 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG11 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG12 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG13 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG21 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG22 | 10       | 0.12          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG23 | 10       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 38       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 38       | 0.12          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 38       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 25       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3  | 39       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2  | 39       | 0.12          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3  | 39       | 0.12          |
| (1,2270) | 1:371:A:ASN:HD21 | 1:374:A:ILE:HD11 | 15       | 0.12          |
| (1,2270) | 1:371:A:ASN:HD21 | 1:374:A:ILE:HD12 | 15       | 0.12          |
| (1,2270) | 1:371:A:ASN:HD21 | 1:374:A:ILE:HD13 | 15       | 0.12          |
| (1,2270) | 1:371:A:ASN:HD22 | 1:374:A:ILE:HD11 | 15       | 0.12          |
| (1,2270) | 1:371:A:ASN:HD22 | 1:374:A:ILE:HD12 | 15       | 0.12          |
| (1,2270) | 1:371:A:ASN:HD22 | 1:374:A:ILE:HD13 | 15       | 0.12          |
| (1,2269) | 1:371:A:ASN:HD21 | 1:374:A:ILE:HG21 | 28       | 0.12          |
| (1,2269) | 1:371:A:ASN:HD21 | 1:374:A:ILE:HG22 | 28       | 0.12          |
| (1,2269) | 1:371:A:ASN:HD21 | 1:374:A:ILE:HG23 | 28       | 0.12          |
| (1,2269) | 1:371:A:ASN:HD22 | 1:374:A:ILE:HG21 | 28       | 0.12          |
| (1,2269) | 1:371:A:ASN:HD22 | 1:374:A:ILE:HG22 | 28       | 0.12          |
| (1,2269) | 1:371:A:ASN:HD22 | 1:374:A:ILE:HG23 | 28       | 0.12          |
| (1,2237) | 1:368:A:LEU:HD11 | 1:369:A:ASP:H    | 28       | 0.12          |
| (1,2237) | 1:368:A:LEU:HD12 | 1:369:A:ASP:H    | 28       | 0.12          |
| (1,2237) | 1:368:A:LEU:HD13 | 1:369:A:ASP:H    | 28       | 0.12          |
| (1,2237) | 1:368:A:LEU:HD21 | 1:369:A:ASP:H    | 28       | 0.12          |
| (1,2237) | 1:368:A:LEU:HD22 | 1:369:A:ASP:H    | 28       | 0.12          |
| (1,2237) | 1:368:A:LEU:HD23 | 1:369:A:ASP:H    | 28       | 0.12          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD11 | 38       | 0.12          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD12 | 38       | 0.12          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD13 | 38       | 0.12          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD21 | 38       | 0.12          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD22 | 38       | 0.12          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD23 | 38       | 0.12          |
| (1,2134) | 1:354:A:ARG:HD2  | 1:357:A:ALA:HB1  | 8        | 0.12          |
| (1,2134) | 1:354:A:ARG:HD2  | 1:357:A:ALA:HB2  | 8        | 0.12          |
| (1,2134) | 1:354:A:ARG:HD2  | 1:357:A:ALA:HB3  | 8        | 0.12          |
| (1,2134) | 1:354:A:ARG:HD3  | 1:357:A:ALA:HB1  | 8        | 0.12          |
| (1,2134) | 1:354:A:ARG:HD3  | 1:357:A:ALA:HB2  | 8        | 0.12          |
| (1,2134) | 1:354:A:ARG:HD3  | 1:357:A:ALA:HB3  | 8        | 0.12          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2077) | 1:348:A:MET:HE1 | 1:385:A:VAL:HG11 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE1 | 1:385:A:VAL:HG12 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE1 | 1:385:A:VAL:HG13 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE1 | 1:385:A:VAL:HG21 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE1 | 1:385:A:VAL:HG22 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE1 | 1:385:A:VAL:HG23 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE2 | 1:385:A:VAL:HG11 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE2 | 1:385:A:VAL:HG12 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE2 | 1:385:A:VAL:HG13 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE2 | 1:385:A:VAL:HG21 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE2 | 1:385:A:VAL:HG22 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE2 | 1:385:A:VAL:HG23 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG11 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG12 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG13 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG21 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG22 | 15       | 0.12          |
| (1,2077) | 1:348:A:MET:HE3 | 1:385:A:VAL:HG23 | 15       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD11 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD12 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD13 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD21 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD22 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD23 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2 | 1:380:A:LEU:HD11 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2 | 1:380:A:LEU:HD12 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2 | 1:380:A:LEU:HD13 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2 | 1:380:A:LEU:HD21 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2 | 1:380:A:LEU:HD22 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2 | 1:380:A:LEU:HD23 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3 | 1:380:A:LEU:HD11 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3 | 1:380:A:LEU:HD12 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3 | 1:380:A:LEU:HD13 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3 | 1:380:A:LEU:HD21 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3 | 1:380:A:LEU:HD22 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3 | 1:380:A:LEU:HD23 | 14       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD11 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD12 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD13 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD21 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD22 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE1 | 1:380:A:LEU:HD23 | 20       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD11 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD12 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD13 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD21 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD22 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD23 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD11 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD12 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD13 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD21 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD22 | 20       | 0.12          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD23 | 20       | 0.12          |
| (1,1809) | 1:429:A:VAL:HG11 | 1:431:A:GLU:H    | 36       | 0.12          |
| (1,1809) | 1:429:A:VAL:HG12 | 1:431:A:GLU:H    | 36       | 0.12          |
| (1,1809) | 1:429:A:VAL:HG13 | 1:431:A:GLU:H    | 36       | 0.12          |
| (1,1809) | 1:429:A:VAL:HG21 | 1:431:A:GLU:H    | 36       | 0.12          |
| (1,1809) | 1:429:A:VAL:HG22 | 1:431:A:GLU:H    | 36       | 0.12          |
| (1,1809) | 1:429:A:VAL:HG23 | 1:431:A:GLU:H    | 36       | 0.12          |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG21 | 9        | 0.12          |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG22 | 9        | 0.12          |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG23 | 9        | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 21       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 26       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 39       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 39       | 0.12          |
| (1,805)  | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 39       | 0.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 39       | 0.12          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 39       | 0.12          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 39       | 0.12          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 39       | 0.12          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 39       | 0.12          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 39       | 0.12          |
| (1,710) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HA   | 15       | 0.12          |
| (1,710) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HA   | 15       | 0.12          |
| (1,710) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HA   | 15       | 0.12          |
| (1,710) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HA   | 17       | 0.12          |
| (1,710) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HA   | 17       | 0.12          |
| (1,710) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HA   | 17       | 0.12          |
| (1,710) | 1:436:A:ILE:HG21 | 1:438:A:GLN:HA   | 18       | 0.12          |
| (1,710) | 1:436:A:ILE:HG22 | 1:438:A:GLN:HA   | 18       | 0.12          |
| (1,710) | 1:436:A:ILE:HG23 | 1:438:A:GLN:HA   | 18       | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 1        | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 1        | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 1        | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 1        | 0.12          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 1        | 0.12          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 1        | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 8        | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 8        | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 8        | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 8        | 0.12          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 8        | 0.12          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 8        | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 24       | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 24       | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 24       | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 24       | 0.12          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 24       | 0.12          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 24       | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 25       | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 25       | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 25       | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 25       | 0.12          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 25       | 0.12          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 25       | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 40       | 0.12          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 40       | 0.12          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 40       | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 40       | 0.12          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 40       | 0.12          |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 40       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 14       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 14       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 14       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 19       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 19       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 19       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 40       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 40       | 0.12          |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 40       | 0.12          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG21 | 28       | 0.12          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG22 | 28       | 0.12          |
| (1,585)  | 1:406:A:PHE:HE1  | 1:412:A:ILE:HG23 | 28       | 0.12          |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG21 | 28       | 0.12          |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG22 | 28       | 0.12          |
| (1,585)  | 1:406:A:PHE:HE2  | 1:412:A:ILE:HG23 | 28       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG11 | 12       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG12 | 12       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG13 | 12       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG11 | 12       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG12 | 12       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG13 | 12       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG11 | 12       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG12 | 12       | 0.12          |
| (1,342)  | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG13 | 12       | 0.12          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1  | 15       | 0.12          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2  | 15       | 0.12          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1  | 15       | 0.12          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2  | 15       | 0.12          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1  | 15       | 0.12          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2  | 15       | 0.12          |
| (1,76)   | 1:355:A:ILE:HD11 | 1:379:A:GLU:HG2  | 5        | 0.12          |
| (1,76)   | 1:355:A:ILE:HD12 | 1:379:A:GLU:HG2  | 5        | 0.12          |
| (1,76)   | 1:355:A:ILE:HD13 | 1:379:A:GLU:HG2  | 5        | 0.12          |
| (1,8)    | 1:343:A:SER:HA   | 1:344:A:TRP:HB2  | 12       | 0.12          |
| (1,8)    | 1:343:A:SER:HA   | 1:344:A:TRP:HB3  | 12       | 0.12          |
| (1,2806) | 1:529:A:PHE:HD1  | 1:533:A:LEU:HD11 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD1  | 1:533:A:LEU:HD12 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD1  | 1:533:A:LEU:HD13 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD1  | 1:533:A:LEU:HD21 | 16       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2806) | 1:529:A:PHE:HD1  | 1:533:A:LEU:HD22 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD1  | 1:533:A:LEU:HD23 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD2  | 1:533:A:LEU:HD11 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD2  | 1:533:A:LEU:HD12 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD2  | 1:533:A:LEU:HD13 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD2  | 1:533:A:LEU:HD21 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD2  | 1:533:A:LEU:HD22 | 16       | 0.11          |
| (1,2806) | 1:529:A:PHE:HD2  | 1:533:A:LEU:HD23 | 16       | 0.11          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 9        | 0.11          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 9        | 0.11          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 14       | 0.11          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 14       | 0.11          |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H    | 15       | 0.11          |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H    | 15       | 0.11          |
| (1,2658) | 1:458:A:LEU:HB2  | 1:459:A:PHE:H    | 5        | 0.11          |
| (1,2658) | 1:458:A:LEU:HB3  | 1:459:A:PHE:H    | 5        | 0.11          |
| (1,2648) | 1:456:A:LYS:H    | 1:456:A:LYS:HB2  | 4        | 0.11          |
| (1,2648) | 1:456:A:LYS:H    | 1:456:A:LYS:HB3  | 4        | 0.11          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD11 | 1        | 0.11          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD12 | 1        | 0.11          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD13 | 1        | 0.11          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD21 | 1        | 0.11          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD22 | 1        | 0.11          |
| (1,2625) | 1:439:A:VAL:H    | 1:440:A:LEU:HD23 | 1        | 0.11          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2  | 11       | 0.11          |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3  | 11       | 0.11          |
| (1,2536) | 1:411:A:VAL:HG11 | 1:412:A:ILE:HB   | 20       | 0.11          |
| (1,2536) | 1:411:A:VAL:HG12 | 1:412:A:ILE:HB   | 20       | 0.11          |
| (1,2536) | 1:411:A:VAL:HG13 | 1:412:A:ILE:HB   | 20       | 0.11          |
| (1,2536) | 1:411:A:VAL:HG21 | 1:412:A:ILE:HB   | 20       | 0.11          |
| (1,2536) | 1:411:A:VAL:HG22 | 1:412:A:ILE:HB   | 20       | 0.11          |
| (1,2536) | 1:411:A:VAL:HG23 | 1:412:A:ILE:HB   | 20       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG11 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG12 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG13 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG21 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG22 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG2  | 1:411:A:VAL:HG23 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG11 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG12 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG13 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG21 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG22 | 20       | 0.11          |
| (1,2530) | 1:410:A:GLN:HG3  | 1:411:A:VAL:HG23 | 20       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 15       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 15       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG11 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG12 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG13 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG21 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG22 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD11 | 1:385:A:VAL:HG23 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG11 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG12 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG13 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG21 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG22 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD12 | 1:385:A:VAL:HG23 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG11 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG12 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG13 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG21 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG22 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD13 | 1:385:A:VAL:HG23 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG11 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG12 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG13 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG21 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG22 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD21 | 1:385:A:VAL:HG23 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG11 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG12 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG13 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG21 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG22 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD22 | 1:385:A:VAL:HG23 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG11 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG12 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG13 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG21 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG22 | 26       | 0.11          |
| (1,2358) | 1:383:A:LEU:HD23 | 1:385:A:VAL:HG23 | 26       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H   | 9        | 0.11          |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H   | 9        | 0.11          |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H   | 9        | 0.11          |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H   | 9        | 0.11          |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H   | 9        | 0.11          |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H   | 9        | 0.11          |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H   | 12       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H   | 12       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H   | 12       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H   | 12       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H   | 12       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H   | 12       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H   | 19       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H   | 19       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H   | 19       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H   | 19       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H   | 19       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H   | 19       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H   | 28       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H   | 28       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H   | 28       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H   | 28       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H   | 28       | 0.11          |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H   | 28       | 0.11          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB1 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB2 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD11 | 1:381:A:ALA:HB3 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB1 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB2 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD12 | 1:381:A:ALA:HB3 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB1 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB2 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD13 | 1:381:A:ALA:HB3 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB1 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB2 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD21 | 1:381:A:ALA:HB3 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB1 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB2 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD22 | 1:381:A:ALA:HB3 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB1 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB2 | 4        | 0.11          |
| (1,2328) | 1:380:A:LEU:HD23 | 1:381:A:ALA:HB3 | 4        | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD1  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD2  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD1  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD2  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD1  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD2  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD1  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD2  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD1  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD2  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD1  | 28       | 0.11          |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD2  | 28       | 0.11          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD11 | 22       | 0.11          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD12 | 22       | 0.11          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD13 | 22       | 0.11          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD21 | 22       | 0.11          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD22 | 22       | 0.11          |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD23 | 22       | 0.11          |
| (1,2221) | 1:365:A:ILE:HG21 | 1:492:A:ASN:HD21 | 2        | 0.11          |
| (1,2221) | 1:365:A:ILE:HG21 | 1:492:A:ASN:HD22 | 2        | 0.11          |
| (1,2221) | 1:365:A:ILE:HG22 | 1:492:A:ASN:HD21 | 2        | 0.11          |
| (1,2221) | 1:365:A:ILE:HG22 | 1:492:A:ASN:HD22 | 2        | 0.11          |
| (1,2221) | 1:365:A:ILE:HG23 | 1:492:A:ASN:HD21 | 2        | 0.11          |
| (1,2221) | 1:365:A:ILE:HG23 | 1:492:A:ASN:HD22 | 2        | 0.11          |
| (1,2097) | 1:352:A:LEU:HG   | 1:380:A:LEU:HD11 | 28       | 0.11          |
| (1,2097) | 1:352:A:LEU:HG   | 1:380:A:LEU:HD12 | 28       | 0.11          |
| (1,2097) | 1:352:A:LEU:HG   | 1:380:A:LEU:HD13 | 28       | 0.11          |
| (1,2097) | 1:352:A:LEU:HG   | 1:380:A:LEU:HD21 | 28       | 0.11          |
| (1,2097) | 1:352:A:LEU:HG   | 1:380:A:LEU:HD22 | 28       | 0.11          |
| (1,2097) | 1:352:A:LEU:HG   | 1:380:A:LEU:HD23 | 28       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD11 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD12 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD13 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD21 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD22 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD23 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD11 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD12 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD13 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD21 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD22 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD23 | 25       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD11 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD12 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD13 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD21 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD22 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD23 | 25       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD11 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD12 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD13 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD21 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD22 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD23 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD11 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD12 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD13 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD21 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD22 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD23 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD11 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD12 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD13 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD21 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD22 | 32       | 0.11          |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD23 | 32       | 0.11          |
| (1,1808) | 1:429:A:VAL:HG11 | 1:432:A:GLY:H    | 20       | 0.11          |
| (1,1808) | 1:429:A:VAL:HG12 | 1:432:A:GLY:H    | 20       | 0.11          |
| (1,1808) | 1:429:A:VAL:HG13 | 1:432:A:GLY:H    | 20       | 0.11          |
| (1,1808) | 1:429:A:VAL:HG21 | 1:432:A:GLY:H    | 20       | 0.11          |
| (1,1808) | 1:429:A:VAL:HG22 | 1:432:A:GLY:H    | 20       | 0.11          |
| (1,1808) | 1:429:A:VAL:HG23 | 1:432:A:GLY:H    | 20       | 0.11          |
| (1,1423) | 1:471:A:ASN:H    | 1:471:A:ASN:HD21 | 12       | 0.11          |
| (1,1092) | 1:471:A:ASN:H    | 1:474:A:ALA:HB1  | 9        | 0.11          |
| (1,1092) | 1:471:A:ASN:H    | 1:474:A:ALA:HB2  | 9        | 0.11          |
| (1,1092) | 1:471:A:ASN:H    | 1:474:A:ALA:HB3  | 9        | 0.11          |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD11 | 3        | 0.11          |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD12 | 3        | 0.11          |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD13 | 3        | 0.11          |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD11 | 3        | 0.11          |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD12 | 3        | 0.11          |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD13 | 3        | 0.11          |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD11 | 12       | 0.11          |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD12 | 12       | 0.11          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,838) | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD13 | 12       | 0.11          |
| (1,838) | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD11 | 12       | 0.11          |
| (1,838) | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD12 | 12       | 0.11          |
| (1,838) | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD13 | 12       | 0.11          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD11 | 34       | 0.11          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD12 | 34       | 0.11          |
| (1,805) | 1:474:A:ALA:HB1  | 1:476:A:ILE:HD13 | 34       | 0.11          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD11 | 34       | 0.11          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD12 | 34       | 0.11          |
| (1,805) | 1:474:A:ALA:HB2  | 1:476:A:ILE:HD13 | 34       | 0.11          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD11 | 34       | 0.11          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD12 | 34       | 0.11          |
| (1,805) | 1:474:A:ALA:HB3  | 1:476:A:ILE:HD13 | 34       | 0.11          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 15       | 0.11          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 15       | 0.11          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 15       | 0.11          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 15       | 0.11          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 15       | 0.11          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 15       | 0.11          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 17       | 0.11          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 17       | 0.11          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 17       | 0.11          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 17       | 0.11          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 17       | 0.11          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 17       | 0.11          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 27       | 0.11          |
| (1,684) | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 27       | 0.11          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 27       | 0.11          |
| (1,684) | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 27       | 0.11          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 27       | 0.11          |
| (1,684) | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 27       | 0.11          |
| (1,682) | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 7        | 0.11          |
| (1,682) | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 7        | 0.11          |
| (1,682) | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 7        | 0.11          |
| (1,682) | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 31       | 0.11          |
| (1,682) | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 31       | 0.11          |
| (1,682) | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 31       | 0.11          |
| (1,632) | 1:417:A:THR:HG21 | 1:418:A:MET:HB2  | 15       | 0.11          |
| (1,632) | 1:417:A:THR:HG21 | 1:418:A:MET:HB3  | 15       | 0.11          |
| (1,632) | 1:417:A:THR:HG22 | 1:418:A:MET:HB2  | 15       | 0.11          |
| (1,632) | 1:417:A:THR:HG22 | 1:418:A:MET:HB3  | 15       | 0.11          |
| (1,632) | 1:417:A:THR:HG23 | 1:418:A:MET:HB2  | 15       | 0.11          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,632)  | 1:417:A:THR:HG23 | 1:418:A:MET:HB3 | 15       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE1 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE2 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE3 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE1 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE2 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE3 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE1 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE2 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE3 | 5        | 0.11          |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE1 | 30       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE2 | 30       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG21 | 1:413:A:MET:HE3 | 30       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE1 | 30       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE2 | 30       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG22 | 1:413:A:MET:HE3 | 30       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE1 | 30       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE2 | 30       | 0.11          |
| (1,588)  | 1:412:A:ILE:HG23 | 1:413:A:MET:HE3 | 30       | 0.11          |
| (1,264)  | 1:381:A:ALA:HB1  | 1:422:A:LYS:HE2 | 2        | 0.11          |
| (1,264)  | 1:381:A:ALA:HB1  | 1:422:A:LYS:HE3 | 2        | 0.11          |
| (1,264)  | 1:381:A:ALA:HB2  | 1:422:A:LYS:HE2 | 2        | 0.11          |
| (1,264)  | 1:381:A:ALA:HB2  | 1:422:A:LYS:HE3 | 2        | 0.11          |
| (1,264)  | 1:381:A:ALA:HB3  | 1:422:A:LYS:HE2 | 2        | 0.11          |
| (1,264)  | 1:381:A:ALA:HB3  | 1:422:A:LYS:HE3 | 2        | 0.11          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1 | 16       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2 | 16       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1 | 16       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2 | 16       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1 | 16       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2 | 16       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE1 | 25       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG21 | 1:406:A:PHE:HE2 | 25       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE1 | 25       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG22 | 1:406:A:PHE:HE2 | 25       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE1 | 25       | 0.11          |
| (1,117)  | 1:359:A:ILE:HG23 | 1:406:A:PHE:HE2 | 25       | 0.11          |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD1 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD11 | 1:529:A:PHE:HD2 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD1 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD12 | 1:529:A:PHE:HD2 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD1 | 20       | 0.1           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2792) | 1:526:A:LEU:HD13 | 1:529:A:PHE:HD2 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD1 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD21 | 1:529:A:PHE:HD2 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD1 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD22 | 1:529:A:PHE:HD2 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD1 | 20       | 0.1           |
| (1,2792) | 1:526:A:LEU:HD23 | 1:529:A:PHE:HD2 | 20       | 0.1           |
| (1,2674) | 1:469:A:GLU:HB2  | 1:470:A:GLU:H   | 11       | 0.1           |
| (1,2674) | 1:469:A:GLU:HB3  | 1:470:A:GLU:H   | 11       | 0.1           |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE2 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG11 | 1:415:A:LYS:HE3 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE2 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG12 | 1:415:A:LYS:HE3 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE2 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG13 | 1:415:A:LYS:HE3 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE2 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG21 | 1:415:A:LYS:HE3 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE2 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG22 | 1:415:A:LYS:HE3 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE2 | 8        | 0.1           |
| (1,2543) | 1:411:A:VAL:HG23 | 1:415:A:LYS:HE3 | 8        | 0.1           |
| (1,2536) | 1:411:A:VAL:HG11 | 1:412:A:ILE:HB  | 6        | 0.1           |
| (1,2536) | 1:411:A:VAL:HG12 | 1:412:A:ILE:HB  | 6        | 0.1           |
| (1,2536) | 1:411:A:VAL:HG13 | 1:412:A:ILE:HB  | 6        | 0.1           |
| (1,2536) | 1:411:A:VAL:HG21 | 1:412:A:ILE:HB  | 6        | 0.1           |
| (1,2536) | 1:411:A:VAL:HG22 | 1:412:A:ILE:HB  | 6        | 0.1           |
| (1,2536) | 1:411:A:VAL:HG23 | 1:412:A:ILE:HB  | 6        | 0.1           |
| (1,2335) | 1:380:A:LEU:HD11 | 1:419:A:LEU:H   | 2        | 0.1           |
| (1,2335) | 1:380:A:LEU:HD12 | 1:419:A:LEU:H   | 2        | 0.1           |
| (1,2335) | 1:380:A:LEU:HD13 | 1:419:A:LEU:H   | 2        | 0.1           |
| (1,2335) | 1:380:A:LEU:HD21 | 1:419:A:LEU:H   | 2        | 0.1           |
| (1,2335) | 1:380:A:LEU:HD22 | 1:419:A:LEU:H   | 2        | 0.1           |
| (1,2335) | 1:380:A:LEU:HD23 | 1:419:A:LEU:H   | 2        | 0.1           |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD1 | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG11 | 1:406:A:PHE:HD2 | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD1 | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG12 | 1:406:A:PHE:HD2 | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD1 | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG13 | 1:406:A:PHE:HD2 | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD1 | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG21 | 1:406:A:PHE:HD2 | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD1 | 22       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2257) | 1:370:A:VAL:HG22 | 1:406:A:PHE:HD2  | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD1  | 22       | 0.1           |
| (1,2257) | 1:370:A:VAL:HG23 | 1:406:A:PHE:HD2  | 22       | 0.1           |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD11 | 8        | 0.1           |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD12 | 8        | 0.1           |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD13 | 8        | 0.1           |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD21 | 8        | 0.1           |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD22 | 8        | 0.1           |
| (1,2226) | 1:367:A:ASN:HA   | 1:368:A:LEU:HD23 | 8        | 0.1           |
| (1,2221) | 1:365:A:ILE:HG21 | 1:492:A:ASN:HD21 | 9        | 0.1           |
| (1,2221) | 1:365:A:ILE:HG21 | 1:492:A:ASN:HD22 | 9        | 0.1           |
| (1,2221) | 1:365:A:ILE:HG22 | 1:492:A:ASN:HD21 | 9        | 0.1           |
| (1,2221) | 1:365:A:ILE:HG22 | 1:492:A:ASN:HD22 | 9        | 0.1           |
| (1,2221) | 1:365:A:ILE:HG23 | 1:492:A:ASN:HD21 | 9        | 0.1           |
| (1,2221) | 1:365:A:ILE:HG23 | 1:492:A:ASN:HD22 | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE1  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE2  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD11 | 1:396:A:MET:HE3  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE1  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE2  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD12 | 1:396:A:MET:HE3  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE1  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE2  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD13 | 1:396:A:MET:HE3  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE1  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE2  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD21 | 1:396:A:MET:HE3  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE1  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE2  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD22 | 1:396:A:MET:HE3  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE1  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE2  | 9        | 0.1           |
| (1,2116) | 1:352:A:LEU:HD23 | 1:396:A:MET:HE3  | 9        | 0.1           |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG11 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG12 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG13 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG21 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG22 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE1  | 1:385:A:VAL:HG23 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG11 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG12 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG13 | 28       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG21 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG22 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE2  | 1:385:A:VAL:HG23 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG11 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG12 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG13 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG21 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG22 | 28       | 0.1           |
| (1,2077) | 1:348:A:MET:HE3  | 1:385:A:VAL:HG23 | 28       | 0.1           |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD11 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD12 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD13 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD21 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD22 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE1  | 1:380:A:LEU:HD23 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD11 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD12 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD13 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD21 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD22 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE2  | 1:380:A:LEU:HD23 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD11 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD12 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD13 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD21 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD22 | 11       | 0.1           |
| (1,2074) | 1:348:A:MET:HE3  | 1:380:A:LEU:HD23 | 11       | 0.1           |
| (1,1809) | 1:429:A:VAL:HG11 | 1:431:A:GLU:H    | 31       | 0.1           |
| (1,1809) | 1:429:A:VAL:HG12 | 1:431:A:GLU:H    | 31       | 0.1           |
| (1,1809) | 1:429:A:VAL:HG13 | 1:431:A:GLU:H    | 31       | 0.1           |
| (1,1809) | 1:429:A:VAL:HG21 | 1:431:A:GLU:H    | 31       | 0.1           |
| (1,1809) | 1:429:A:VAL:HG22 | 1:431:A:GLU:H    | 31       | 0.1           |
| (1,1809) | 1:429:A:VAL:HG23 | 1:431:A:GLU:H    | 31       | 0.1           |
| (1,1343) | 1:463:A:SER:H    | 1:463:A:SER:HB2  | 6        | 0.1           |
| (1,1343) | 1:463:A:SER:H    | 1:463:A:SER:HB3  | 6        | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG21 | 3        | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG22 | 3        | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG23 | 3        | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG21 | 11       | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG22 | 11       | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG23 | 11       | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG21 | 12       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG22 | 12       | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG23 | 12       | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG21 | 22       | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG22 | 22       | 0.1           |
| (1,1052) | 1:407:A:LYS:H    | 1:412:A:ILE:HG23 | 22       | 0.1           |
| (1,965)  | 1:385:A:VAL:HB   | 1:423:A:PHE:HE1  | 28       | 0.1           |
| (1,965)  | 1:385:A:VAL:HB   | 1:423:A:PHE:HE2  | 28       | 0.1           |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD11 | 6        | 0.1           |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD12 | 6        | 0.1           |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD13 | 6        | 0.1           |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD11 | 6        | 0.1           |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD12 | 6        | 0.1           |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD13 | 6        | 0.1           |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD11 | 40       | 0.1           |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD12 | 40       | 0.1           |
| (1,838)  | 1:427:A:PHE:HE1  | 1:476:A:ILE:HD13 | 40       | 0.1           |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD11 | 40       | 0.1           |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD12 | 40       | 0.1           |
| (1,838)  | 1:427:A:PHE:HE2  | 1:476:A:ILE:HD13 | 40       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 7        | 0.1           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 7        | 0.1           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 7        | 0.1           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 7        | 0.1           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 7        | 0.1           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 7        | 0.1           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 31       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 31       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 31       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 31       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 31       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 31       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD1  | 32       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD11 | 1:477:A:PHE:HD2  | 32       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD1  | 32       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD12 | 1:477:A:PHE:HD2  | 32       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD1  | 32       | 0.1           |
| (1,684)  | 1:428:A:LEU:HD13 | 1:477:A:PHE:HD2  | 32       | 0.1           |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD21 | 23       | 0.1           |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD22 | 23       | 0.1           |
| (1,682)  | 1:526:A:LEU:HA   | 1:526:A:LEU:HD23 | 23       | 0.1           |
| (1,610)  | 1:348:A:MET:HE1  | 1:352:A:LEU:HG   | 8        | 0.1           |
| (1,610)  | 1:348:A:MET:HE2  | 1:352:A:LEU:HG   | 8        | 0.1           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,610) | 1:348:A:MET:HE3  | 1:352:A:LEU:HG   | 8        | 0.1           |
| (1,610) | 1:348:A:MET:HE1  | 1:352:A:LEU:HG   | 16       | 0.1           |
| (1,610) | 1:348:A:MET:HE2  | 1:352:A:LEU:HG   | 16       | 0.1           |
| (1,610) | 1:348:A:MET:HE3  | 1:352:A:LEU:HG   | 16       | 0.1           |
| (1,610) | 1:348:A:MET:HE1  | 1:352:A:LEU:HG   | 31       | 0.1           |
| (1,610) | 1:348:A:MET:HE2  | 1:352:A:LEU:HG   | 31       | 0.1           |
| (1,610) | 1:348:A:MET:HE3  | 1:352:A:LEU:HG   | 31       | 0.1           |
| (1,342) | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG11 | 16       | 0.1           |
| (1,342) | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG12 | 16       | 0.1           |
| (1,342) | 1:352:A:LEU:HD21 | 1:385:A:VAL:HG13 | 16       | 0.1           |
| (1,342) | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG11 | 16       | 0.1           |
| (1,342) | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG12 | 16       | 0.1           |
| (1,342) | 1:352:A:LEU:HD22 | 1:385:A:VAL:HG13 | 16       | 0.1           |
| (1,342) | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG11 | 16       | 0.1           |
| (1,342) | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG12 | 16       | 0.1           |
| (1,342) | 1:352:A:LEU:HD23 | 1:385:A:VAL:HG13 | 16       | 0.1           |
| (1,192) | 1:365:A:ILE:HD11 | 1:491:A:PHE:HA   | 5        | 0.1           |
| (1,192) | 1:365:A:ILE:HD12 | 1:491:A:PHE:HA   | 5        | 0.1           |
| (1,192) | 1:365:A:ILE:HD13 | 1:491:A:PHE:HA   | 5        | 0.1           |

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

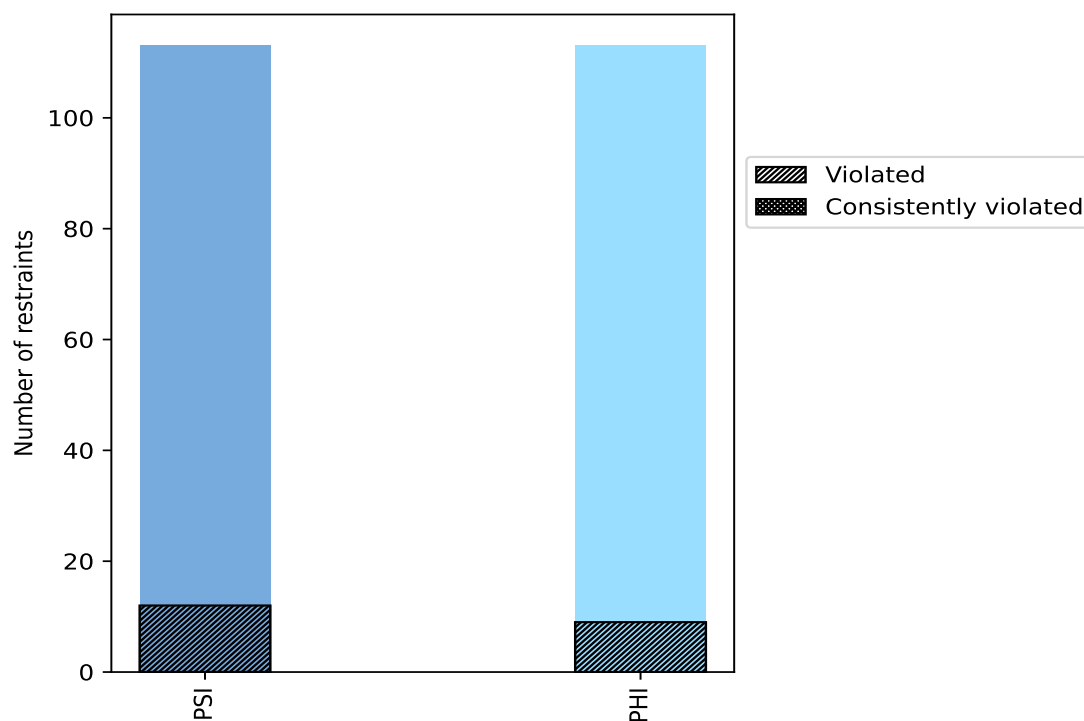
### 10.1 Summary of dihedral-angle violations [i](#)

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        | 113   | 50.0           | 12                    | 10.6           | 5.3            | 0                                  | 0.0            | 0.0            |
| PHI        | 113   | 50.0           | 9                     | 8.0            | 4.0            | 0                                  | 0.0            | 0.0            |
| Total      | 226   | 100.0          | 21                    | 9.3            | 9.3            | 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.

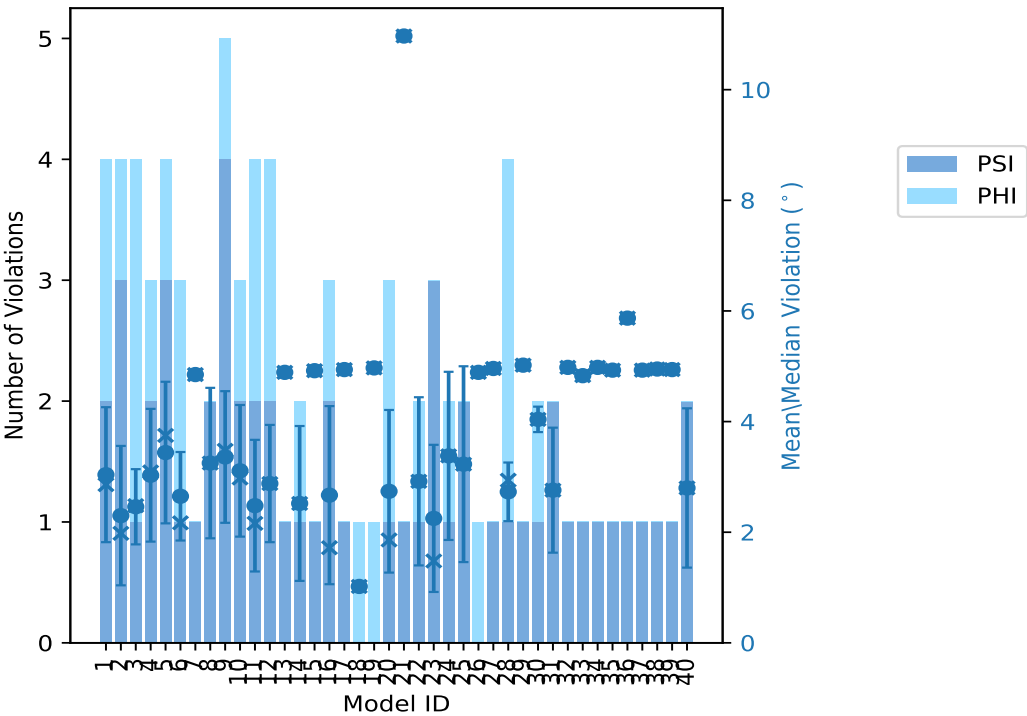
| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 2                    | 2   | 4     | 3.04     | 4.92    | 1.22   | 2.86       |
| 2        | 3                    | 1   | 4     | 2.3      | 4.22    | 1.26   | 1.98       |
| 3        | 1                    | 3   | 4     | 2.46     | 3.2     | 0.68   | 2.48       |
| 4        | 2                    | 1   | 3     | 3.03     | 4.47    | 1.2    | 3.09       |
| 5        | 3                    | 1   | 4     | 3.44     | 4.89    | 1.28   | 3.75       |
| 6        | 1                    | 2   | 3     | 2.65     | 3.78    | 0.8    | 2.17       |
| 7        | 1                    | 0   | 1     | 4.85     | 4.85    | 0.0    | 4.85       |
| 8        | 2                    | 0   | 2     | 3.25     | 4.61    | 1.36   | 3.25       |
| 9        | 4                    | 1   | 5     | 3.36     | 4.68    | 1.19   | 3.48       |
| 10       | 2                    | 1   | 3     | 3.11     | 4.63    | 1.19   | 2.98       |
| 11       | 2                    | 2   | 4     | 2.48     | 4.38    | 1.19   | 2.16       |
| 12       | 2                    | 2   | 4     | 2.88     | 4.39    | 1.06   | 2.88       |
| 13       | 1                    | 0   | 1     | 4.89     | 4.89    | 0.0    | 4.89       |
| 14       | 1                    | 1   | 2     | 2.52     | 3.91    | 1.4    | 2.52       |
| 15       | 1                    | 0   | 1     | 4.92     | 4.92    | 0.0    | 4.92       |
| 16       | 2                    | 1   | 3     | 2.67     | 4.94    | 1.61   | 1.72       |
| 17       | 1                    | 0   | 1     | 4.94     | 4.94    | 0.0    | 4.94       |
| 18       | 0                    | 1   | 1     | 1.02     | 1.02    | 0.0    | 1.02       |
| 19       | 0                    | 1   | 1     | 4.97     | 4.97    | 0.0    | 4.97       |
| 20       | 1                    | 2   | 3     | 2.74     | 4.81    | 1.47   | 1.86       |
| 21       | 1                    | 0   | 1     | 10.97    | 10.97   | 0.0    | 10.97      |
| 22       | 1                    | 1   | 2     | 2.92     | 4.43    | 1.52   | 2.92       |
| 23       | 3                    | 0   | 3     | 2.25     | 4.12    | 1.33   | 1.48       |
| 24       | 1                    | 1   | 2     | 3.38     | 4.9     | 1.52   | 3.38       |
| 25       | 2                    | 0   | 2     | 3.23     | 5.0     | 1.77   | 3.23       |
| 26       | 0                    | 1   | 1     | 4.89     | 4.89    | 0.0    | 4.89       |
| 27       | 1                    | 0   | 1     | 4.96     | 4.96    | 0.0    | 4.96       |
| 28       | 1                    | 3   | 4     | 2.73     | 3.18    | 0.53   | 2.94       |
| 29       | 1                    | 0   | 1     | 5.02     | 5.02    | 0.0    | 5.02       |
| 30       | 1                    | 1   | 2     | 4.04     | 4.27    | 0.23   | 4.04       |
| 31       | 2                    | 0   | 2     | 2.76     | 3.89    | 1.13   | 2.76       |
| 32       | 1                    | 0   | 1     | 4.98     | 4.98    | 0.0    | 4.98       |
| 33       | 1                    | 0   | 1     | 4.83     | 4.83    | 0.0    | 4.83       |
| 34       | 1                    | 0   | 1     | 4.98     | 4.98    | 0.0    | 4.98       |
| 35       | 1                    | 0   | 1     | 4.93     | 4.93    | 0.0    | 4.93       |
| 36       | 1                    | 0   | 1     | 5.87     | 5.87    | 0.0    | 5.87       |
| 37       | 1                    | 0   | 1     | 4.93     | 4.93    | 0.0    | 4.93       |
| 38       | 1                    | 0   | 1     | 4.95     | 4.95    | 0.0    | 4.95       |

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| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 39       | 1                    | 0   | 1     | 4.94     | 4.94    | 0.0    | 4.94       |
| 40       | 2                    | 0   | 2     | 2.8      | 4.24    | 1.44   | 2.8        |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 5                             | 4   | 9     | 1                        | 2.5  |
| 2                             | 2   | 4     | 2                        | 5.0  |
| 1                             | 0   | 1     | 3                        | 7.5  |
| 0                             | 0   | 0     | 4                        | 10.0 |

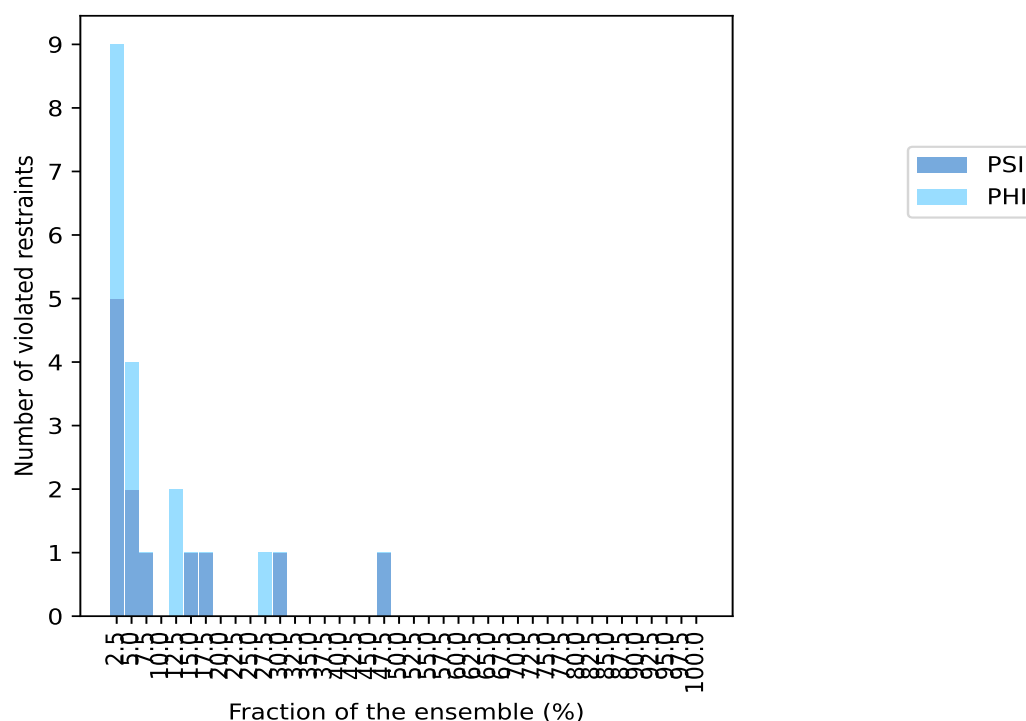
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 2   | 2     | 5                        | 12.5  |
| 1                             | 0   | 1     | 6                        | 15.0  |
| 1                             | 0   | 1     | 7                        | 17.5  |
| 0                             | 0   | 0     | 8                        | 20.0  |
| 0                             | 0   | 0     | 9                        | 22.5  |
| 0                             | 0   | 0     | 10                       | 25.0  |
| 0                             | 1   | 1     | 11                       | 27.5  |
| 1                             | 0   | 1     | 12                       | 30.0  |
| 0                             | 0   | 0     | 13                       | 32.5  |
| 0                             | 0   | 0     | 14                       | 35.0  |
| 0                             | 0   | 0     | 15                       | 37.5  |
| 0                             | 0   | 0     | 16                       | 40.0  |
| 0                             | 0   | 0     | 17                       | 42.5  |
| 0                             | 0   | 0     | 18                       | 45.0  |
| 1                             | 0   | 1     | 19                       | 47.5  |
| 0                             | 0   | 0     | 20                       | 50.0  |
| 0                             | 0   | 0     | 21                       | 52.5  |
| 0                             | 0   | 0     | 22                       | 55.0  |
| 0                             | 0   | 0     | 23                       | 57.5  |
| 0                             | 0   | 0     | 24                       | 60.0  |
| 0                             | 0   | 0     | 25                       | 62.5  |
| 0                             | 0   | 0     | 26                       | 65.0  |
| 0                             | 0   | 0     | 27                       | 67.5  |
| 0                             | 0   | 0     | 28                       | 70.0  |
| 0                             | 0   | 0     | 29                       | 72.5  |
| 0                             | 0   | 0     | 30                       | 75.0  |
| 0                             | 0   | 0     | 31                       | 77.5  |
| 0                             | 0   | 0     | 32                       | 80.0  |
| 0                             | 0   | 0     | 33                       | 82.5  |
| 0                             | 0   | 0     | 34                       | 85.0  |
| 0                             | 0   | 0     | 35                       | 87.5  |
| 0                             | 0   | 0     | 36                       | 90.0  |
| 0                             | 0   | 0     | 37                       | 92.5  |
| 0                             | 0   | 0     | 38                       | 95.0  |
| 0                             | 0   | 0     | 39                       | 97.5  |
| 0                             | 0   | 0     | 40                       | 100.0 |

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

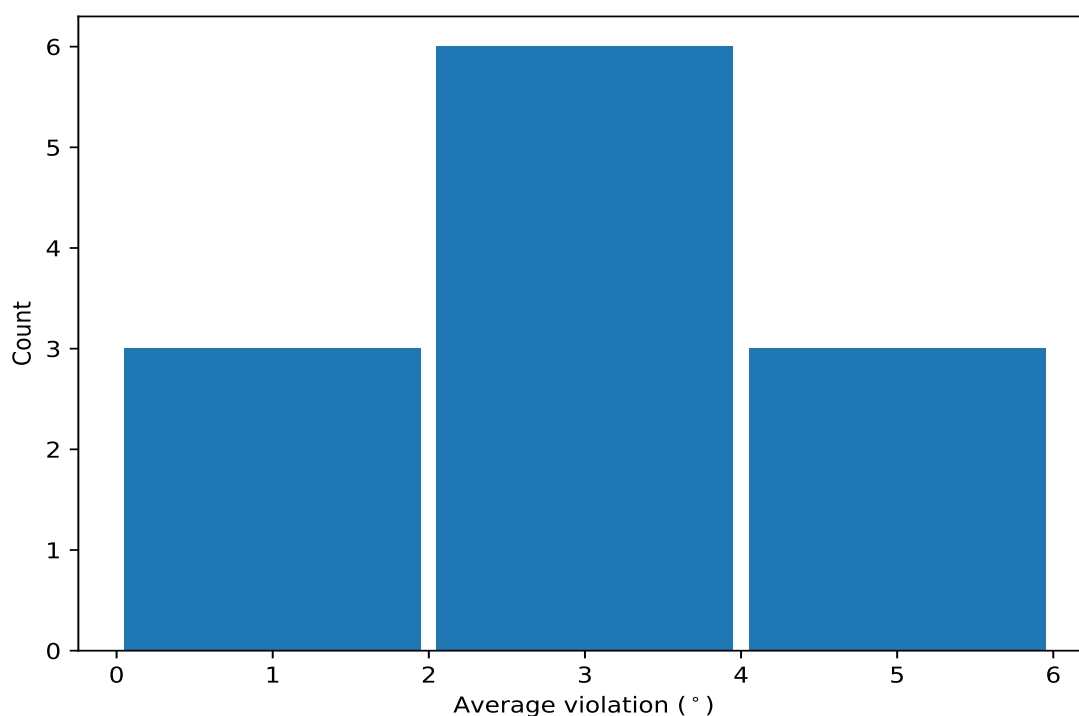
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



#### 10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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.

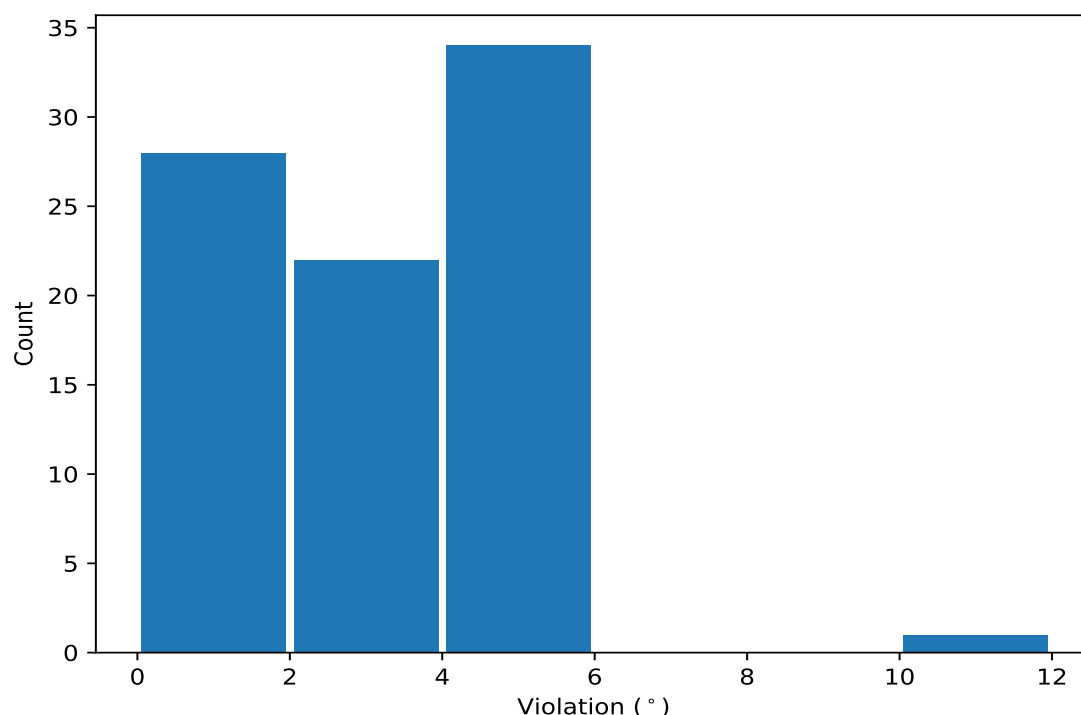
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 19                  | 4.21 | 0.65            | 4.38   |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 12                  | 5.01 | 0.26            | 4.94   |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 11                  | 2.16 | 1.09            | 1.87   |
| (1,116) | 1:411:A:VAL:N | 1:411:A:VAL:CA | 1:411:A:VAL:C  | 1:412:A:ILE:N | 7                   | 3.0  | 1.11            | 3.09   |
| (1,140) | 1:423:A:PHE:N | 1:423:A:PHE:CA | 1:423:A:PHE:C  | 1:424:A:LYS:N | 6                   | 2.01 | 1.15            | 1.5    |
| (1,151) | 1:467:A:ASN:C | 1:468:A:GLU:N  | 1:468:A:GLU:CA | 1:468:A:GLU:C | 5                   | 4.34 | 0.72            | 4.81   |
| (1,85)  | 1:394:A:THR:C | 1:395:A:GLU:N  | 1:395:A:GLU:CA | 1:395:A:GLU:C | 5                   | 2.07 | 0.75            | 1.99   |
| (1,172) | 1:478:A:GLY:N | 1:478:A:GLY:CA | 1:478:A:GLY:C  | 1:479:A:GLU:N | 3                   | 3.2  | 1.58            | 3.48   |
| (1,10)  | 1:350:A:SER:N | 1:350:A:SER:CA | 1:350:A:SER:C  | 1:351:A:ARG:N | 2                   | 2.25 | 0.36            | 2.25   |
| (1,73)  | 1:388:A:GLN:C | 1:389:A:GLN:N  | 1:389:A:GLN:CA | 1:389:A:GLN:C | 2                   | 1.68 | 0.14            | 1.68   |
| (1,143) | 1:424:A:LYS:C | 1:425:A:ASN:N  | 1:425:A:ASN:CA | 1:425:A:ASN:C | 2                   | 1.54 | 0.15            | 1.54   |
| (1,212) | 1:532:A:MET:N | 1:532:A:MET:CA | 1:532:A:MET:C  | 1:533:A:LEU:N | 2                   | 1.53 | 0.19            | 1.53   |

<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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,204) | 1:528:A:ASP:N | 1:528:A:ASP:CA | 1:528:A:ASP:C  | 1:529:A:PHE:N | 21       | 10.97         |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 36       | 5.87          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 29       | 5.02          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 25       | 5.0           |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 34       | 4.98          |
| (1,172) | 1:478:A:GLY:N | 1:478:A:GLY:CA | 1:478:A:GLY:C  | 1:479:A:GLU:N | 32       | 4.98          |
| (1,151) | 1:467:A:ASN:C | 1:468:A:GLU:N  | 1:468:A:GLU:CA | 1:468:A:GLU:C | 19       | 4.97          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 27       | 4.96          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 38       | 4.95          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 16       | 4.94          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 17       | 4.94          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 39       | 4.94          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 35       | 4.93          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 37       | 4.93          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 15       | 4.92          |
| (1,151) | 1:467:A:ASN:C | 1:468:A:GLU:N  | 1:468:A:GLU:CA | 1:468:A:GLU:C | 1        | 4.92          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 24       | 4.9           |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 13       | 4.89          |
| (1,177) | 1:483:A:GLU:C | 1:484:A:GLU:N  | 1:484:A:GLU:CA | 1:484:A:GLU:C | 26       | 4.89          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 5        | 4.89          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 7        | 4.85          |
| (1,178) | 1:484:A:GLU:N | 1:484:A:GLU:CA | 1:484:A:GLU:C  | 1:485:A:GLU:N | 33       | 4.83          |
| (1,151) | 1:467:A:ASN:C | 1:468:A:GLU:N  | 1:468:A:GLU:CA | 1:468:A:GLU:C | 20       | 4.81          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 9        | 4.68          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 10       | 4.63          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 8        | 4.61          |
| (1,140) | 1:423:A:PHE:N | 1:423:A:PHE:CA | 1:423:A:PHE:C  | 1:424:A:LYS:N | 9        | 4.58          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 4        | 4.47          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 22       | 4.43          |
| (1,116) | 1:411:A:VAL:N | 1:411:A:VAL:CA | 1:411:A:VAL:C  | 1:412:A:ILE:N | 12       | 4.39          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 11       | 4.38          |
| (1,116) | 1:411:A:VAL:N | 1:411:A:VAL:CA | 1:411:A:VAL:C  | 1:412:A:ILE:N | 30       | 4.27          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 40       | 4.24          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 2        | 4.22          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 23       | 4.12          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 14       | 3.91          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 31       | 3.89          |
| (1,170) | 1:477:A:PHE:N | 1:477:A:PHE:CA | 1:477:A:PHE:C  | 1:478:A:GLY:N | 5        | 3.82          |
| (1,151) | 1:467:A:ASN:C | 1:468:A:GLU:N  | 1:468:A:GLU:CA | 1:468:A:GLU:C | 30       | 3.81          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 6        | 3.78          |
| (1,116) | 1:411:A:VAL:N | 1:411:A:VAL:CA | 1:411:A:VAL:C  | 1:412:A:ILE:N | 5        | 3.68          |
| (1,172) | 1:478:A:GLY:N | 1:478:A:GLY:CA | 1:478:A:GLY:C  | 1:479:A:GLU:N | 9        | 3.48          |
| (1,145) | 1:425:A:ASN:C | 1:426:A:MET:N  | 1:426:A:MET:CA | 1:426:A:MET:C | 3        | 3.2           |
| (1,151) | 1:467:A:ASN:C | 1:468:A:GLU:N  | 1:468:A:GLU:CA | 1:468:A:GLU:C | 28       | 3.18          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 28       | 3.13          |
| (1,116) | 1:411:A:VAL:N | 1:411:A:VAL:CA | 1:411:A:VAL:C  | 1:412:A:ILE:N | 4        | 3.09          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 3        | 3.08          |
| (1,85)  | 1:394:A:THR:C | 1:395:A:GLU:N  | 1:395:A:GLU:CA | 1:395:A:GLU:C | 10       | 2.98          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 1        | 2.92          |
| (1,85)  | 1:394:A:THR:C | 1:395:A:GLU:N  | 1:395:A:GLU:CA | 1:395:A:GLU:C | 12       | 2.88          |
| (1,182) | 1:489:A:THR:N | 1:489:A:THR:CA | 1:489:A:THR:C  | 1:490:A:GLY:N | 12       | 2.87          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 1        | 2.81          |
| (1,8)   | 1:349:A:ASP:N | 1:349:A:ASP:CA | 1:349:A:ASP:C  | 1:350:A:SER:N | 28       | 2.75          |
| (1,10)  | 1:350:A:SER:N | 1:350:A:SER:CA | 1:350:A:SER:C  | 1:351:A:ARG:N | 2        | 2.61          |
| (1,116) | 1:411:A:VAL:N | 1:411:A:VAL:CA | 1:411:A:VAL:C  | 1:412:A:ILE:N | 11       | 2.5           |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 9        | 2.38          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 6        | 2.17          |
| (1,85)  | 1:394:A:THR:C | 1:395:A:GLU:N  | 1:395:A:GLU:CA | 1:395:A:GLU:C | 6        | 1.99          |
| (1,10)  | 1:350:A:SER:N | 1:350:A:SER:CA | 1:350:A:SER:C  | 1:351:A:ARG:N | 8        | 1.89          |
| (1,211) | 1:531:A:MET:C | 1:532:A:MET:N  | 1:532:A:MET:CA | 1:532:A:MET:C | 3        | 1.87          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 24       | 1.87          |
| (1,6)   | 1:348:A:MET:N | 1:348:A:MET:CA | 1:348:A:MET:C  | 1:349:A:ASP:N | 20       | 1.86          |
| (1,41)  | 1:370:A:VAL:C | 1:371:A:ASN:N  | 1:371:A:ASN:CA | 1:371:A:ASN:C | 28       | 1.85          |
| (1,73)  | 1:388:A:GLN:C | 1:389:A:GLN:N  | 1:389:A:GLN:CA | 1:389:A:GLN:C | 11       | 1.81          |
| (1,212) | 1:532:A:MET:N | 1:532:A:MET:CA | 1:532:A:MET:C  | 1:533:A:LEU:N | 10       | 1.72          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 16       | 1.72          |
| (1,143) | 1:424:A:LYS:C | 1:425:A:ASN:N  | 1:425:A:ASN:CA | 1:425:A:ASN:C | 3        | 1.69          |
| (1,116) | 1:411:A:VAL:N | 1:411:A:VAL:CA | 1:411:A:VAL:C  | 1:412:A:ILE:N | 9        | 1.67          |
| (1,140) | 1:423:A:PHE:N | 1:423:A:PHE:CA | 1:423:A:PHE:C  | 1:424:A:LYS:N | 31       | 1.63          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 20       | 1.54          |
| (1,73)  | 1:388:A:GLN:C | 1:389:A:GLN:N  | 1:389:A:GLN:CA | 1:389:A:GLN:C | 4        | 1.54          |
| (1,140) | 1:423:A:PHE:N | 1:423:A:PHE:CA | 1:423:A:PHE:C  | 1:424:A:LYS:N | 1        | 1.52          |
| (1,140) | 1:423:A:PHE:N | 1:423:A:PHE:CA | 1:423:A:PHE:C  | 1:424:A:LYS:N | 23       | 1.48          |
| (1,140) | 1:423:A:PHE:N | 1:423:A:PHE:CA | 1:423:A:PHE:C  | 1:424:A:LYS:N | 25       | 1.46          |
| (1,143) | 1:424:A:LYS:C | 1:425:A:ASN:N  | 1:425:A:ASN:CA | 1:425:A:ASN:C | 12       | 1.4           |
| (1,85)  | 1:394:A:THR:C | 1:395:A:GLU:N  | 1:395:A:GLU:CA | 1:395:A:GLU:C | 22       | 1.4           |
| (1,140) | 1:423:A:PHE:N | 1:423:A:PHE:CA | 1:423:A:PHE:C  | 1:424:A:LYS:N | 5        | 1.39          |
| (1,116) | 1:411:A:VAL:N | 1:411:A:VAL:CA | 1:411:A:VAL:C  | 1:412:A:ILE:N | 40       | 1.37          |
| (1,208) | 1:530:A:GLU:N | 1:530:A:GLU:CA | 1:530:A:GLU:C  | 1:531:A:MET:N | 16       | 1.35          |
| (1,212) | 1:532:A:MET:N | 1:532:A:MET:CA | 1:532:A:MET:C  | 1:533:A:LEU:N | 2        | 1.34          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 11       | 1.21          |
| (1,172) | 1:478:A:GLY:N | 1:478:A:GLY:CA | 1:478:A:GLY:C  | 1:479:A:GLU:N | 23       | 1.14          |
| (1,85)  | 1:394:A:THR:C | 1:395:A:GLU:N  | 1:395:A:GLU:CA | 1:395:A:GLU:C | 14       | 1.12          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 18       | 1.02          |
| (1,139) | 1:422:A:LYS:C | 1:423:A:PHE:N  | 1:423:A:PHE:CA | 1:423:A:PHE:C | 2        | 1.01          |