



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:32 PM UTC

PDB ID : 7DAB / pdb\_00007dab  
BMRB ID : 36391  
Title : plant peptide hormone  
Authors : Umetsu, Y.; Ohki, S.  
Deposited on : 2020-10-16

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

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

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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

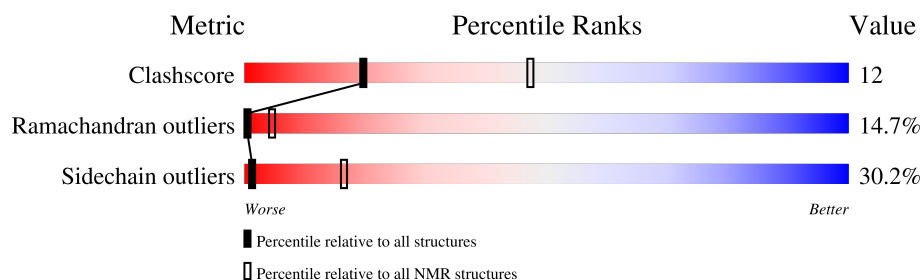
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 34%.

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     | 64     | <div> <div></div> <div>23%</div> <div>25%</div> <div>5%</div> <div>47%</div> </div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:21-A:25, A:31-A:59 (34) | 0.52              | 8            |

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 3 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 922 atoms, of which 450 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Maternally expressed gene14.

| Mol | Chain | Residues | Atoms |     |     |    |    |   |  | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|--|-------|
| 1   | A     | 64       | Total | C   | H   | N  | O  | S |  | 0     |
|     |       |          | 922   | 284 | 450 | 86 | 93 | 9 |  |       |

There is a discrepancy between the modelled and reference sequences:

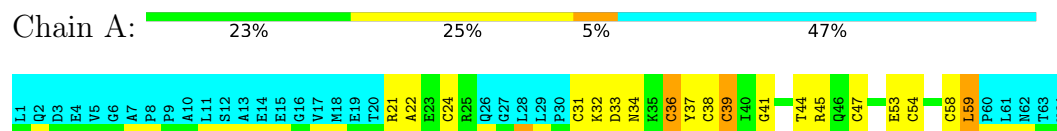
| Chain | Residue | Modelled | Actual | Comment | Reference      |
|-------|---------|----------|--------|---------|----------------|
| A     | 27      | GLY      | VAL    | variant | UNP A0A076YHT9 |

## 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: Maternally expressed gene14

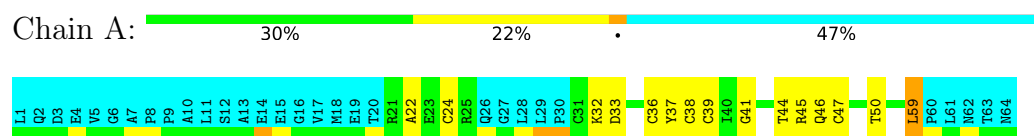


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

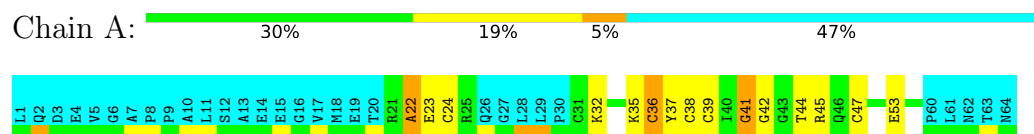
#### 4.2.1 Score per residue for model 1

- Molecule 1: Maternally expressed gene14



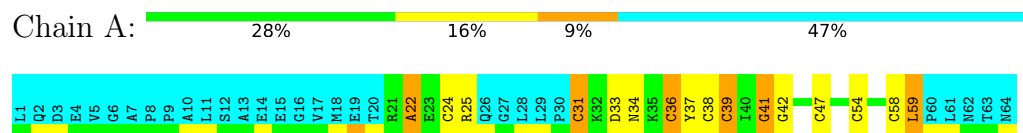
#### 4.2.2 Score per residue for model 2

- Molecule 1: Maternally expressed gene14



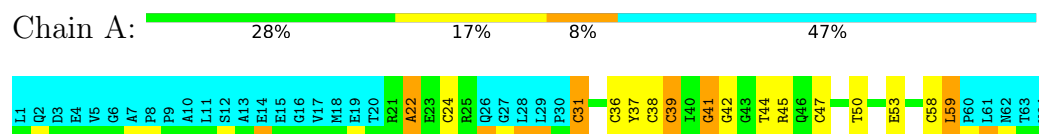
### 4.2.3 Score per residue for model 3

- Molecule 1: Maternally expressed gene14



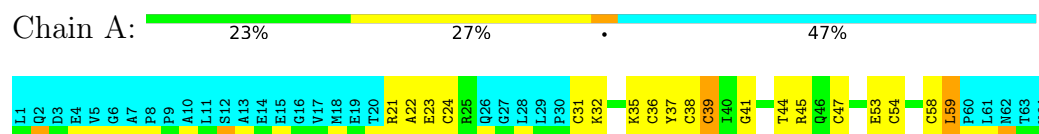
### 4.2.4 Score per residue for model 4

- Molecule 1: Maternally expressed gene14



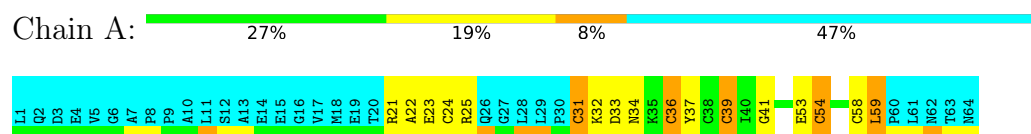
### 4.2.5 Score per residue for model 5

- Molecule 1: Maternally expressed gene14



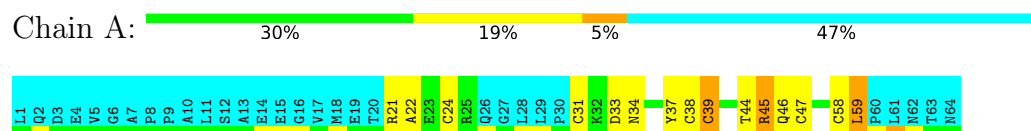
### 4.2.6 Score per residue for model 6

- Molecule 1: Maternally expressed gene14



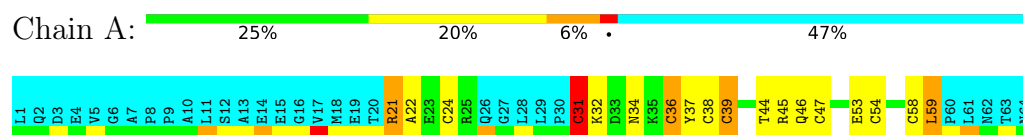
### 4.2.7 Score per residue for model 7

- Molecule 1: Maternally expressed gene14



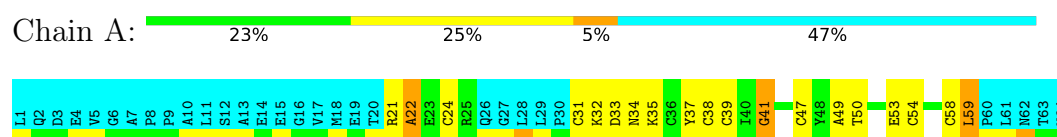
### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Maternally expressed gene14



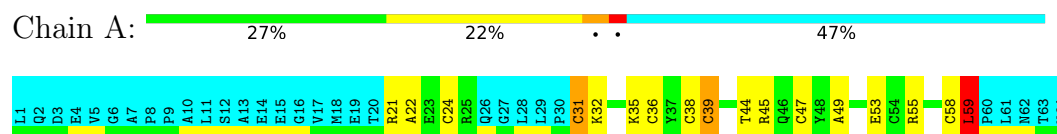
### 4.2.9 Score per residue for model 9

- Molecule 1: Maternally expressed gene14



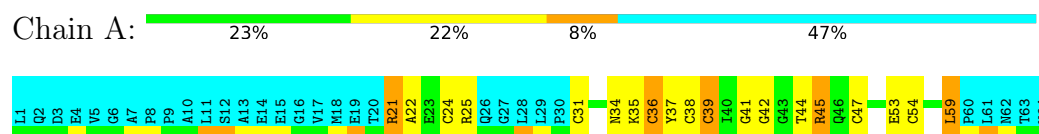
### 4.2.10 Score per residue for model 10

- Molecule 1: Maternally expressed gene14



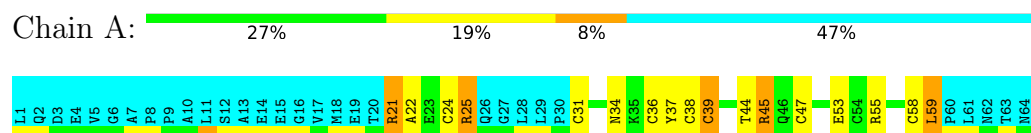
### 4.2.11 Score per residue for model 11

- Molecule 1: Maternally expressed gene14



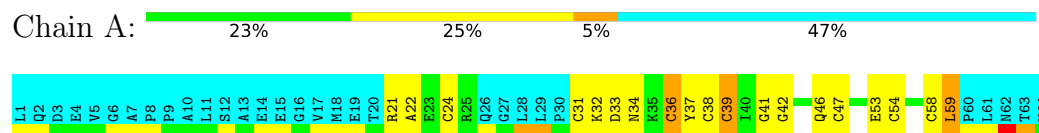
### 4.2.12 Score per residue for model 12

- Molecule 1: Maternally expressed gene14



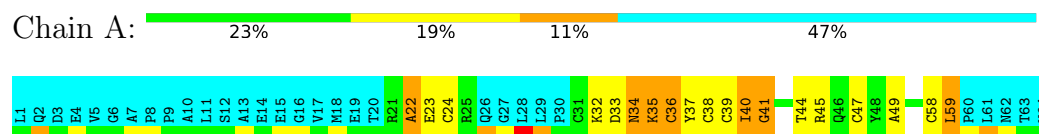
### 4.2.13 Score per residue for model 13

- Molecule 1: Maternally expressed gene14



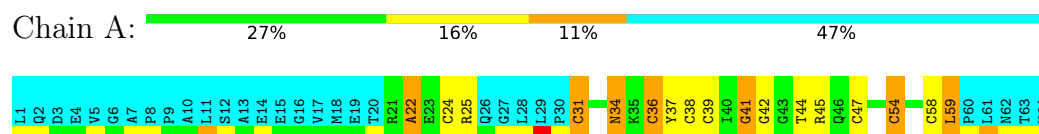
### 4.2.14 Score per residue for model 14

- Molecule 1: Maternally expressed gene14



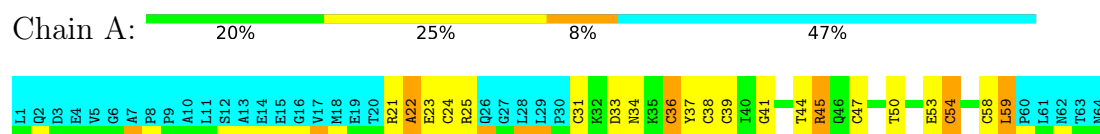
### 4.2.15 Score per residue for model 15

- Molecule 1: Maternally expressed gene14



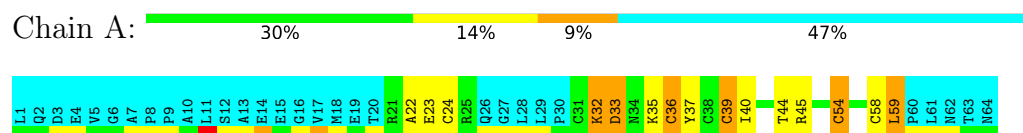
### 4.2.16 Score per residue for model 16

- Molecule 1: Maternally expressed gene14



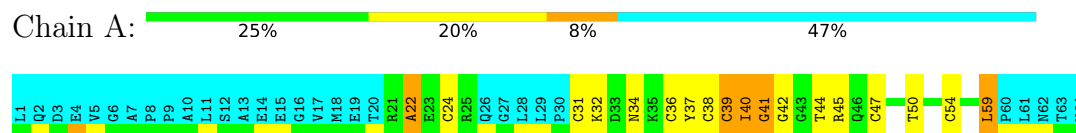
### 4.2.17 Score per residue for model 17

- Molecule 1: Maternally expressed gene14



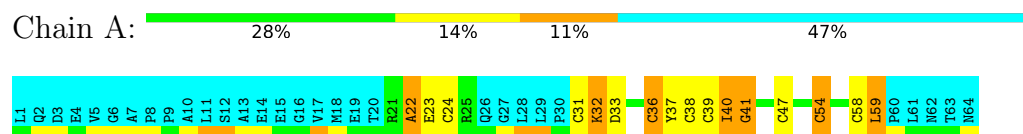
### 4.2.18 Score per residue for model 18

- Molecule 1: Maternally expressed gene14



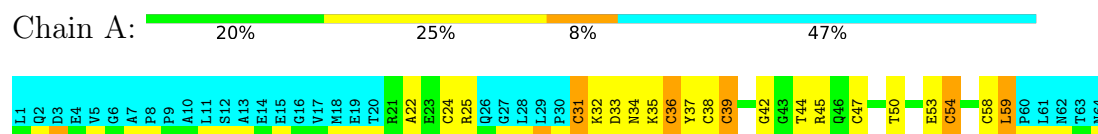
### 4.2.19 Score per residue for model 19

- Molecule 1: Maternally expressed gene14



### 4.2.20 Score per residue for model 20

- Molecule 1: Maternally expressed gene14



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CYANA         | structure calculation |         |

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               | 2              |
| Total number of shifts                       | 558            |
| Number of shifts mapped to atoms             | 558            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 34%            |

## 6 Model quality [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [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     | 257   | 241      | 247      | 6±2     |
| All | All   | 5140  | 4820     | 4893     | 125     |

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 12.

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

| Atom-1         | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|----------------|-----------------|----------|-------------|--------|-------|
|                |                 |          |             | Worst  | Total |
| 1:A:38:CYS:SG  | 1:A:47:CYS:SG   | 1.38     | 1.43        | 5      | 18    |
| 1:A:31:CYS:SG  | 1:A:36:CYS:SG   | 1.28     | 2.32        | 19     | 7     |
| 1:A:36:CYS:CB  | 1:A:54:CYS:SG   | 1.00     | 2.48        | 16     | 8     |
| 1:A:38:CYS:SG  | 1:A:47:CYS:CB   | 0.95     | 2.54        | 10     | 16    |
| 1:A:38:CYS:CB  | 1:A:47:CYS:SG   | 0.95     | 2.55        | 10     | 15    |
| 1:A:36:CYS:SG  | 1:A:54:CYS:CB   | 0.93     | 2.56        | 11     | 2     |
| 1:A:24:CYS:CB  | 1:A:39:CYS:SG   | 0.89     | 2.60        | 3      | 12    |
| 1:A:24:CYS:SG  | 1:A:39:CYS:CB   | 0.85     | 2.64        | 3      | 2     |
| 1:A:38:CYS:HG  | 1:A:47:CYS:CB   | 0.79     | 1.90        | 8      | 2     |
| 1:A:58:CYS:O   | 1:A:59:LEU:HD23 | 0.61     | 1.96        | 10     | 1     |
| 1:A:39:CYS:C   | 1:A:40:ILE:HD13 | 0.56     | 2.25        | 17     | 1     |
| 1:A:22:ALA:HB3 | 1:A:41:GLY:HA2  | 0.55     | 1.78        | 19     | 10    |
| 1:A:58:CYS:C   | 1:A:59:LEU:HD23 | 0.52     | 2.29        | 10     | 1     |
| 1:A:21:ARG:HD3 | 1:A:44:THR:HG21 | 0.51     | 1.82        | 16     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:22:ALA:HB3  | 1:A:41:GLY:CA   | 0.50     | 2.36        | 19     | 5     |
| 1:A:35:LYS:HA   | 1:A:49:ALA:HB2  | 0.49     | 1.84        | 10     | 2     |
| 1:A:44:THR:O    | 1:A:45:ARG:C    | 0.47     | 2.58        | 7      | 15    |
| 1:A:34:ASN:O    | 1:A:49:ALA:HB1  | 0.47     | 2.10        | 9      | 1     |
| 1:A:55:ARG:HA   | 1:A:59:LEU:HD21 | 0.43     | 1.90        | 12     | 1     |
| 1:A:21:ARG:NE   | 1:A:44:THR:HG21 | 0.42     | 2.28        | 12     | 1     |
| 1:A:55:ARG:O    | 1:A:59:LEU:HD11 | 0.42     | 2.13        | 10     | 1     |
| 1:A:40:ILE:O    | 1:A:40:ILE:HD12 | 0.41     | 2.15        | 19     | 1     |
| 1:A:40:ILE:HD12 | 1:A:40:ILE:O    | 0.40     | 2.16        | 14     | 2     |

## 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     | 34/64 (53%)    | 22±1 (64±4%) | 7±1 (21±4%) | 5±1 (15±4%) | 0           | 4 |
| All | All   | 680/1280 (53%) | 437 (64%)    | 143 (21%)   | 100 (15%)   | 0           | 4 |

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 22  | ALA  | 19             |
| 1   | A     | 36  | CYS  | 18             |
| 1   | A     | 58  | CYS  | 15             |
| 1   | A     | 41  | GLY  | 12             |
| 1   | A     | 34  | ASN  | 9              |
| 1   | A     | 42  | GLY  | 8              |
| 1   | A     | 31  | CYS  | 5              |
| 1   | A     | 33  | ASP  | 4              |
| 1   | A     | 32  | LYS  | 4              |
| 1   | A     | 21  | ARG  | 3              |
| 1   | A     | 35  | LYS  | 2              |
| 1   | A     | 59  | LEU  | 1              |

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

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

| Mol | Chain | Analysed       | Rotameric    | Outliers    | Percentiles |    |
|-----|-------|----------------|--------------|-------------|-------------|----|
| 1   | A     | 27/51 (53%)    | 19±2 (70±6%) | 8±2 (30±6%) | 1           | 16 |
| All | All   | 540/1020 (53%) | 377 (70%)    | 163 (30%)   | 1           | 16 |

All 18 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     | 39  | CYS  | 20             |
| 1   | A     | 37  | TYR  | 19             |
| 1   | A     | 59  | LEU  | 19             |
| 1   | A     | 53  | GLU  | 12             |
| 1   | A     | 31  | CYS  | 12             |
| 1   | A     | 32  | LYS  | 11             |
| 1   | A     | 54  | CYS  | 11             |
| 1   | A     | 33  | ASP  | 8              |
| 1   | A     | 21  | ARG  | 8              |
| 1   | A     | 24  | CYS  | 7              |
| 1   | A     | 23  | GLU  | 7              |
| 1   | A     | 50  | THR  | 6              |
| 1   | A     | 35  | LYS  | 5              |
| 1   | A     | 34  | ASN  | 5              |
| 1   | A     | 46  | GLN  | 4              |
| 1   | A     | 45  | ARG  | 4              |
| 1   | A     | 40  | ILE  | 3              |
| 1   | A     | 25  | ARG  | 2              |

### 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 34% for the well-defined parts and 35% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 279 |
| Number of shifts mapped to atoms        | 279 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 57       | $2.66 \pm 0.17$                 | Should be applied          |
| $^{13}\text{C}_\beta$  | 50       | $2.67 \pm 0.31$                 | Should be applied          |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 53       | $-0.03 \pm 0.31$                | None needed ( $< 0.5$ ppm) |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 34%, i.e. 148 atoms were assigned a chemical shift out of a possible 431. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|--------------|-----------------|-----------------|
| Backbone  | 122/173 (71%) | 63/71 (89%)  | 30/68 (44%)     | 29/34 (85%)     |
| Sidechain | 26/233 (11%)  | 0/149 (0%)   | 26/68 (38%)     | 0/16 (0%)       |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 0/25 (0%)     | 0/12 (0%)      | 0/12 (0%)       | 0/1 (0%)        |
| Overall  | 148/431 (34%) | 63/232 (27%)   | 56/148 (38%)    | 29/51 (57%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 278 atoms were assigned a chemical shift out of a possible 800. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 228/318 (72%) | 118/130 (91%)  | 57/128 (45%)    | 53/60 (88%)     |
| Sidechain | 50/457 (11%)  | 0/296 (0%)     | 50/141 (35%)    | 0/20 (0%)       |
| Aromatic  | 0/25 (0%)     | 0/12 (0%)      | 0/12 (0%)       | 0/1 (0%)        |
| Overall   | 278/800 (35%) | 118/438 (27%)  | 107/281 (38%)   | 53/81 (65%)     |

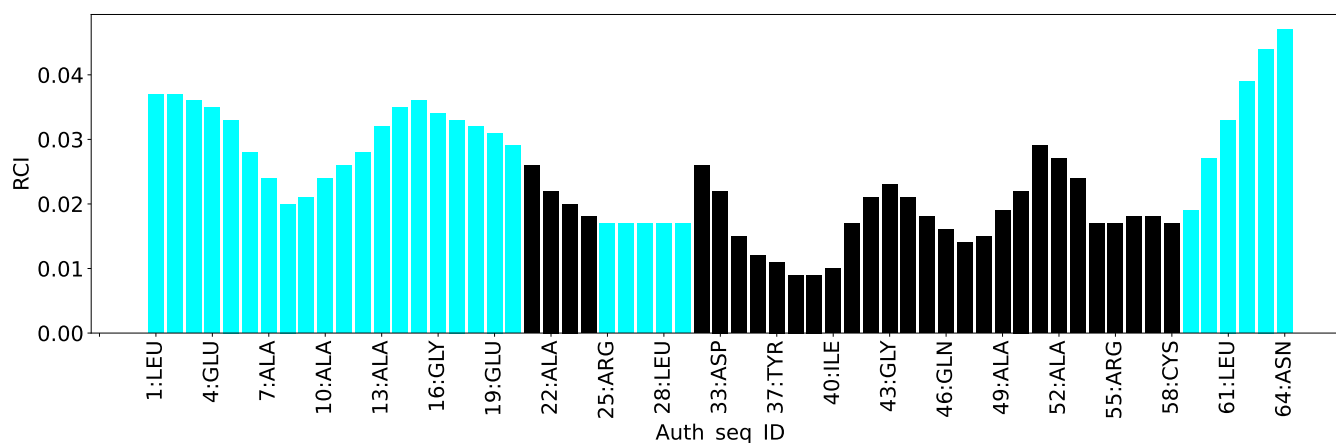
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: working\_cs.cif

Chemical shift list name: *D\_1300019000\_cs\_P1.str.V1\_starch\_output*

### 7.2.1 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                  | 279 |
| Number of shifts mapped to atoms        | 279 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

### 7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 57       | $2.66 \pm 0.17$                 | Should be applied          |
| $^{13}\text{C}_\beta$  | 50       | $2.67 \pm 0.31$                 | Should be applied          |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 53       | $-0.03 \pm 0.31$                | None needed ( $< 0.5$ ppm) |

### 7.2.3 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 34%, i.e. 148 atoms were assigned a chemical shift out of a possible 431. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|--------------|-----------------|-----------------|
| Backbone  | 122/173 (71%) | 63/71 (89%)  | 30/68 (44%)     | 29/34 (85%)     |
| Sidechain | 26/233 (11%)  | 0/149 (0%)   | 26/68 (38%)     | 0/16 (0%)       |
| Aromatic  | 0/25 (0%)     | 0/12 (0%)    | 0/12 (0%)       | 0/1 (0%)        |
| Overall   | 148/431 (34%) | 63/232 (27%) | 56/148 (38%)    | 29/51 (57%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 278 atoms were assigned a chemical shift out of a possible 800. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 228/318 (72%) | 118/130 (91%)  | 57/128 (45%)    | 53/60 (88%)     |
| Sidechain | 50/457 (11%)  | 0/296 (0%)     | 50/141 (35%)    | 0/20 (0%)       |
| Aromatic  | 0/25 (0%)     | 0/12 (0%)      | 0/12 (0%)       | 0/1 (0%)        |
| Overall   | 278/800 (35%) | 118/438 (27%)  | 107/281 (38%)   | 53/81 (65%)     |

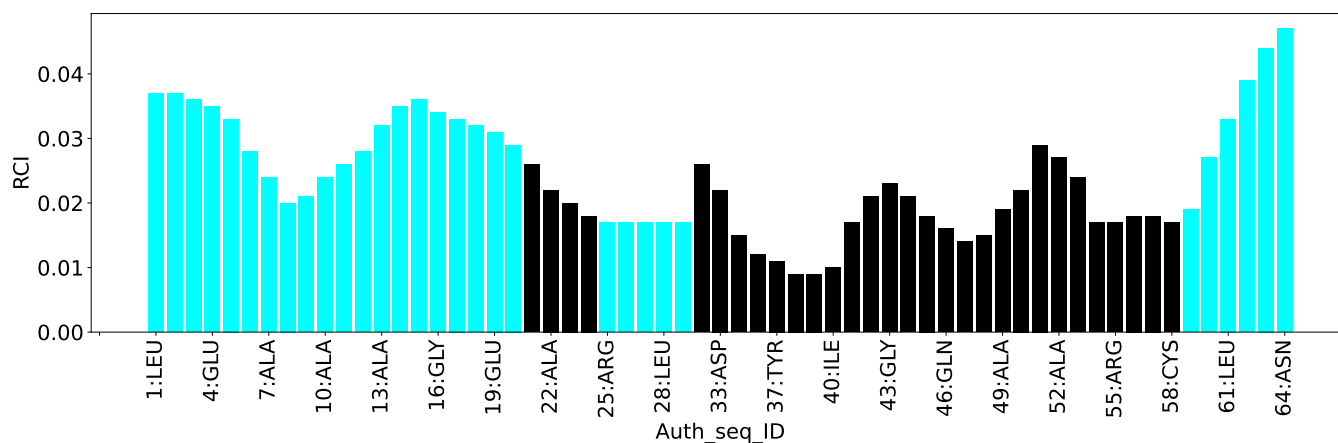
## 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 392   |
| Intra-residue ( $ i-j =0$ )                              | 111   |
| Sequential ( $ i-j =1$ )                                 | 150   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 57    |
| Long range ( $ i-j \geq 5$ )                             | 74    |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 0     |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 6.1   |
| Number of long range restraints per residue <sup>1</sup> | 1.2   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 9.6                                    | 0.2     |
| 0.2-0.5 (Medium) | 10.7                                   | 0.5     |
| >0.5 (Large)     | 14.1                                   | 7.77    |

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

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

## 9 Distance violation analysis ⓘ

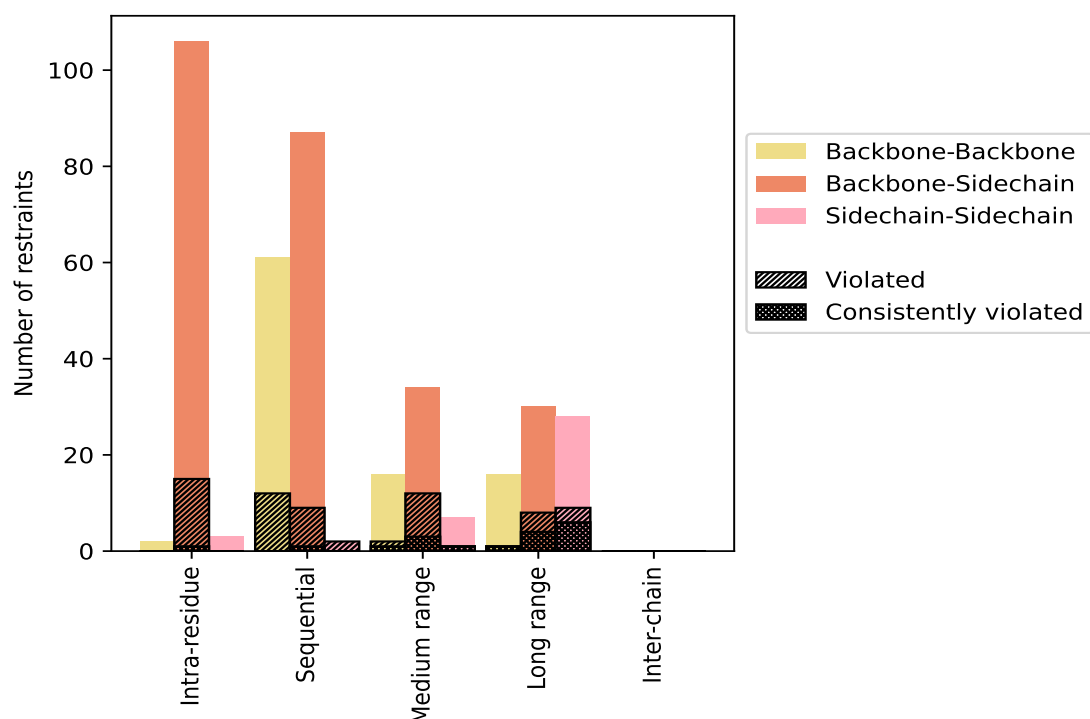
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                             | Count               | % <sup>1</sup>        | Violated <sup>3</sup> |                      |                      | Consistently Violated <sup>4</sup> |                      |                     |
|------------------------------------------------------------|---------------------|-----------------------|-----------------------|----------------------|----------------------|------------------------------------|----------------------|---------------------|
|                                                            |                     |                       | Count                 | % <sup>2</sup>       | % <sup>1</sup>       | Count                              | % <sup>2</sup>       | % <sup>1</sup>      |
| <a href="#">Intra-residue ( i-j =0)</a>                    | <a href="#">111</a> | <a href="#">28.3</a>  | <a href="#">15</a>    | <a href="#">13.5</a> | <a href="#">3.8</a>  | <a href="#">1</a>                  | <a href="#">0.9</a>  | <a href="#">0.3</a> |
| Backbone-Backbone                                          | 2                   | 0.5                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 106                 | 27.0                  | 15                    | 14.2                 | 3.8                  | 1                                  | 0.9                  | 0.3                 |
| Sidechain-Sidechain                                        | 3                   | 0.8                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">150</a> | <a href="#">38.3</a>  | <a href="#">23</a>    | <a href="#">15.3</a> | <a href="#">5.9</a>  | <a href="#">1</a>                  | <a href="#">0.7</a>  | <a href="#">0.3</a> |
| Backbone-Backbone                                          | 61                  | 15.6                  | 12                    | 19.7                 | 3.1                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 87                  | 22.2                  | 9                     | 10.3                 | 2.3                  | 1                                  | 1.1                  | 0.3                 |
| Sidechain-Sidechain                                        | 2                   | 0.5                   | 2                     | 100.0                | 0.5                  | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">57</a>  | <a href="#">14.5</a>  | <a href="#">15</a>    | <a href="#">26.3</a> | <a href="#">3.8</a>  | <a href="#">5</a>                  | <a href="#">8.8</a>  | <a href="#">1.3</a> |
| Backbone-Backbone                                          | 16                  | 4.1                   | 2                     | 12.5                 | 0.5                  | 1                                  | 6.2                  | 0.3                 |
| Backbone-Sidechain                                         | 34                  | 8.7                   | 12                    | 35.3                 | 3.1                  | 3                                  | 8.8                  | 0.8                 |
| Sidechain-Sidechain                                        | 7                   | 1.8                   | 1                     | 14.3                 | 0.3                  | 1                                  | 14.3                 | 0.3                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">74</a>  | <a href="#">18.9</a>  | <a href="#">18</a>    | <a href="#">24.3</a> | <a href="#">4.6</a>  | <a href="#">11</a>                 | <a href="#">14.9</a> | <a href="#">2.8</a> |
| Backbone-Backbone                                          | 16                  | 4.1                   | 1                     | 6.2                  | 0.3                  | 1                                  | 6.2                  | 0.3                 |
| Backbone-Sidechain                                         | 30                  | 7.7                   | 8                     | 26.7                 | 2.0                  | 4                                  | 13.3                 | 1.0                 |
| Sidechain-Sidechain                                        | 28                  | 7.1                   | 9                     | 32.1                 | 2.3                  | 6                                  | 21.4                 | 1.5                 |
| <a href="#">Inter-chain</a>                                | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Backbone-Sidechain                                         | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| Sidechain-Sidechain                                        | 0                   | 0.0                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                  | 0.0                 |
| <a href="#">Hydrogen bond</a>                              | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Disulfide bond</a>                             | <a href="#">0</a>   | <a href="#">0.0</a>   | <a href="#">0</a>     | <a href="#">0.0</a>  | <a href="#">0.0</a>  | <a href="#">0</a>                  | <a href="#">0.0</a>  | <a href="#">0.0</a> |
| <a href="#">Total</a>                                      | <a href="#">392</a> | <a href="#">100.0</a> | <a href="#">71</a>    | <a href="#">18.1</a> | <a href="#">18.1</a> | <a href="#">18</a>                 | <a href="#">4.6</a>  | <a href="#">4.6</a> |
| Backbone-Backbone                                          | 95                  | 24.2                  | 15                    | 15.8                 | 3.8                  | 2                                  | 2.1                  | 0.5                 |
| Backbone-Sidechain                                         | 257                 | 65.6                  | 44                    | 17.1                 | 11.2                 | 9                                  | 3.5                  | 2.3                 |
| Sidechain-Sidechain                                        | 40                  | 10.2                  | 12                    | 30.0                 | 3.1                  | 7                                  | 17.5                 | 1.8                 |

<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        | 5                    | 5               | 10              | 14              | 0               | 34    | 1.16     | 4.75    | 1.4                 | 0.45       |
| 2        | 3                    | 8               | 11              | 14              | 0               | 36    | 1.28     | 5.18    | 1.52                | 0.48       |
| 3        | 2                    | 7               | 7               | 14              | 0               | 30    | 1.14     | 5.56    | 1.49                | 0.32       |
| 4        | 4                    | 9               | 8               | 15              | 0               | 36    | 1.22     | 6.67    | 1.67                | 0.32       |
| 5        | 3                    | 7               | 8               | 15              | 0               | 33    | 1.22     | 6.45    | 1.62                | 0.3        |
| 6        | 4                    | 10              | 8               | 15              | 0               | 37    | 1.12     | 7.0     | 1.59                | 0.29       |
| 7        | 2                    | 8               | 8               | 14              | 0               | 32    | 1.28     | 6.93    | 1.7                 | 0.34       |
| 8        | 6                    | 7               | 8               | 14              | 0               | 35    | 1.12     | 7.49    | 1.63                | 0.3        |
| 9        | 3                    | 8               | 8               | 14              | 0               | 33    | 1.23     | 6.57    | 1.62                | 0.31       |
| 10       | 5                    | 7               | 10              | 14              | 0               | 36    | 0.93     | 4.45    | 1.23                | 0.3        |

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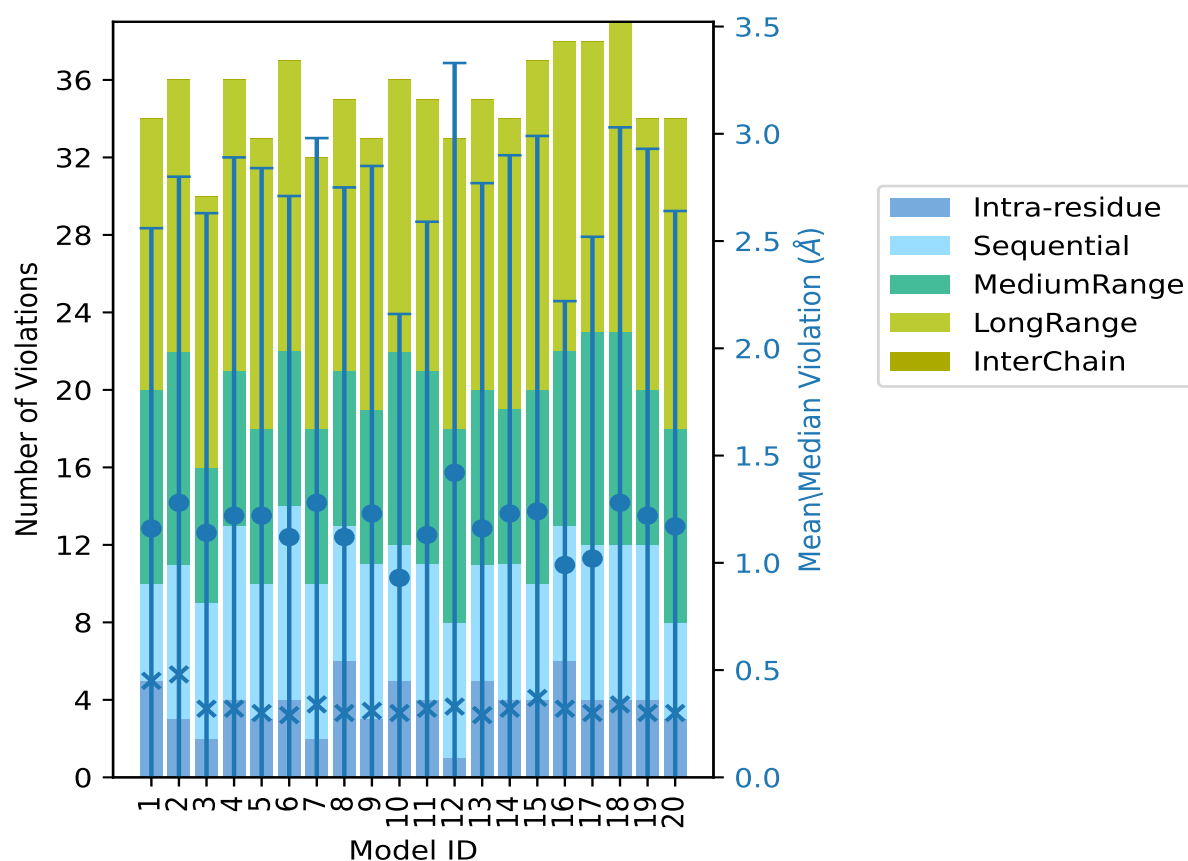
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 4                    | 7               | 10              | 14              | 0               | 35    | 1.13     | 6.34    | 1.46                | 0.32       |
| 12       | 1                    | 7               | 10              | 15              | 0               | 33    | 1.42     | 7.39    | 1.91                | 0.33       |
| 13       | 5                    | 6               | 9               | 15              | 0               | 35    | 1.16     | 6.93    | 1.61                | 0.29       |
| 14       | 4                    | 7               | 8               | 15              | 0               | 34    | 1.23     | 6.52    | 1.67                | 0.32       |
| 15       | 4                    | 6               | 10              | 17              | 0               | 37    | 1.24     | 7.21    | 1.75                | 0.37       |
| 16       | 6                    | 7               | 9               | 16              | 0               | 38    | 0.99     | 4.55    | 1.23                | 0.32       |
| 17       | 4                    | 8               | 11              | 15              | 0               | 38    | 1.02     | 6.28    | 1.5                 | 0.3        |
| 18       | 4                    | 8               | 11              | 16              | 0               | 39    | 1.28     | 6.95    | 1.75                | 0.34       |
| 19       | 4                    | 8               | 8               | 14              | 0               | 34    | 1.22     | 7.77    | 1.71                | 0.3        |
| 20       | 3                    | 5               | 10              | 16              | 0               | 34    | 1.17     | 5.26    | 1.47                | 0.3        |

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

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

### 9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

### 9.3 Distance violation statistics for the ensemble

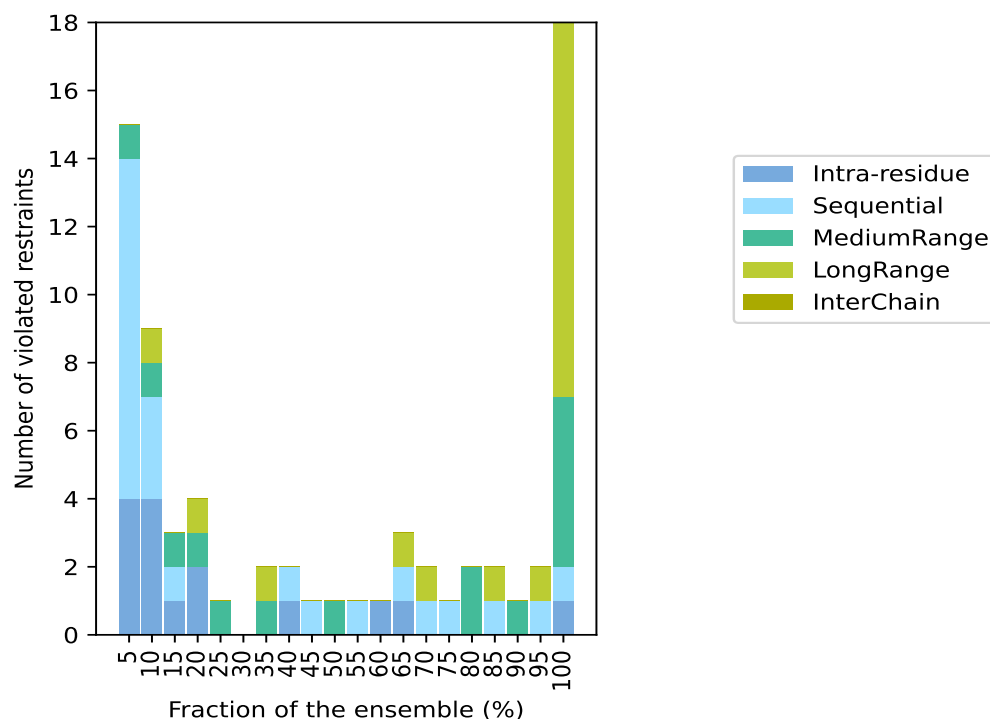
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 321(IR:96, SQ:127, MR:42, LR:56, IC:0) restraints are not 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>       | %     |
| 4                             | 10              | 1               | 0               | 0               | 15    | 1                        | 5.0   |
| 4                             | 3               | 1               | 1               | 0               | 9     | 2                        | 10.0  |
| 1                             | 1               | 1               | 0               | 0               | 3     | 3                        | 15.0  |
| 2                             | 0               | 1               | 1               | 0               | 4     | 4                        | 20.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 5                        | 25.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 6                        | 30.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 7                        | 35.0  |
| 1                             | 1               | 0               | 0               | 0               | 2     | 8                        | 40.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 9                        | 45.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 10                       | 50.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 11                       | 55.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 12                       | 60.0  |
| 1                             | 1               | 0               | 1               | 0               | 3     | 13                       | 65.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 14                       | 70.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 15                       | 75.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 16                       | 80.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 17                       | 85.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 18                       | 90.0  |
| 0                             | 1               | 0               | 1               | 0               | 2     | 19                       | 95.0  |
| 1                             | 1               | 5               | 11              | 0               | 18    | 20                       | 100.0 |

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

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

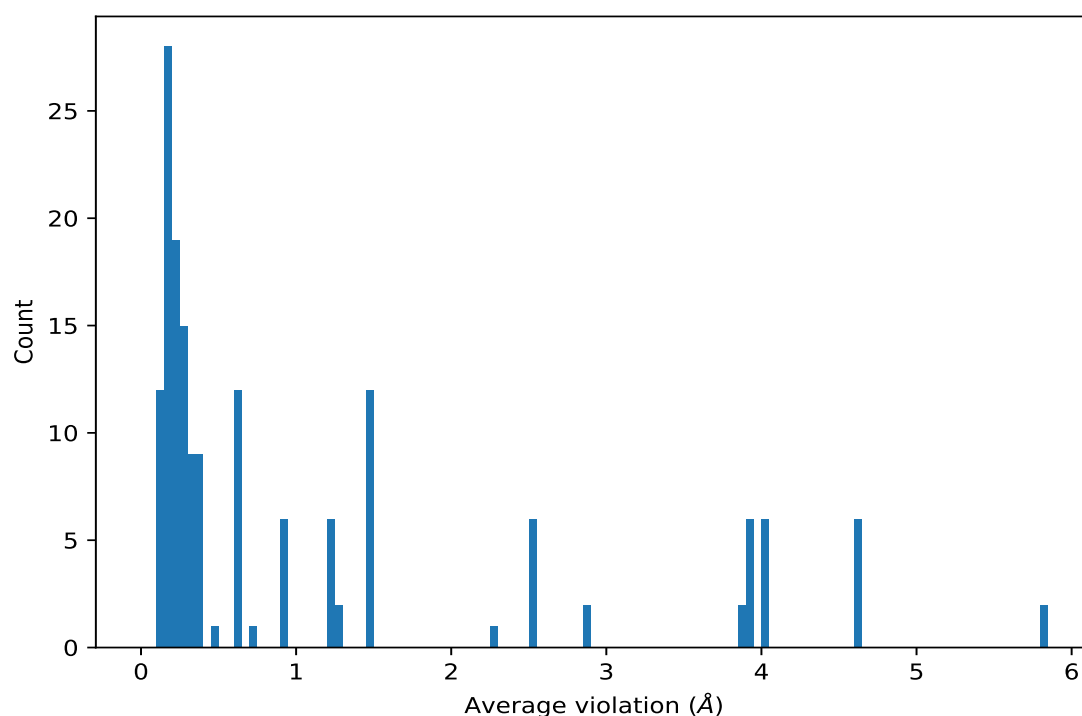
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 20                  | 5.8      | 1.9                 | 6.54       |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 20                  | 5.8      | 1.9                 | 6.54       |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 20                  | 4.61     | 0.13                | 4.58       |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 20                  | 4.61     | 0.13                | 4.58       |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 20                  | 4.61     | 0.13                | 4.58       |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 20                  | 4.61     | 0.13                | 4.58       |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 20                  | 4.61     | 0.13                | 4.58       |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 20                  | 4.61     | 0.13                | 4.58       |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 20                  | 4.0      | 0.19                | 3.98       |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 20                  | 4.0      | 0.19                | 3.98       |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 20                  | 4.0      | 0.19                | 3.98       |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 20                  | 4.0      | 0.19                | 3.98       |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 20                  | 4.0      | 0.19                | 3.98       |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 20                  | 4.0      | 0.19                | 3.98       |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 20                  | 3.93     | 0.62                | 3.81       |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 20                  | 3.93     | 0.62                | 3.81       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 20                  | 3.93     | 0.62                | 3.81       |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 20                  | 3.93     | 0.62                | 3.81       |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 20                  | 3.93     | 0.62                | 3.81       |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 20                  | 3.93     | 0.62                | 3.81       |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 20                  | 3.86     | 0.91                | 3.69       |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 20                  | 3.86     | 0.91                | 3.69       |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA   | 20                  | 2.86     | 0.17                | 2.84       |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA   | 20                  | 2.86     | 0.17                | 2.84       |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H    | 20                  | 2.53     | 0.43                | 2.54       |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H    | 20                  | 2.53     | 0.43                | 2.54       |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H    | 20                  | 2.53     | 0.43                | 2.54       |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H    | 20                  | 2.53     | 0.43                | 2.54       |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H    | 20                  | 2.53     | 0.43                | 2.54       |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H    | 20                  | 2.53     | 0.43                | 2.54       |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H    | 20                  | 2.27     | 0.5                 | 2.44       |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 20                  | 1.49     | 0.77                | 1.32       |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 20                  | 1.21     | 0.14                | 1.23       |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 20                  | 1.21     | 0.14                | 1.23       |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 20                  | 1.21     | 0.14                | 1.23       |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 20                  | 1.2      | 0.01                | 1.2        |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 20                  | 1.2      | 0.01                | 1.2        |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 20                  | 1.2      | 0.01                | 1.2        |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 20                  | 0.38     | 0.02                | 0.37       |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 20                  | 0.38     | 0.02                | 0.37       |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 20                  | 0.38     | 0.02                | 0.37       |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 20                  | 0.3      | 0.02                | 0.3        |
| (1,58)  | 1:21:A:ARG:HB2  | 1:39:A:CYS:HB3  | 20                  | 0.3      | 0.05                | 0.32       |
| (1,58)  | 1:21:A:ARG:HB3  | 1:39:A:CYS:HB3  | 20                  | 0.3      | 0.05                | 0.32       |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 20                  | 0.26     | 0.03                | 0.26       |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 20                  | 0.26     | 0.03                | 0.26       |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 20                  | 0.23     | 0.02                | 0.23       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 20                  | 0.23     | 0.02                | 0.23       |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 20                  | 0.23     | 0.02                | 0.23       |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 20                  | 0.17     | 0.03                | 0.18       |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 20                  | 0.14     | 0.01                | 0.14       |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 20                  | 0.14     | 0.01                | 0.14       |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 20                  | 0.14     | 0.01                | 0.14       |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 19                  | 0.63     | 0.17                | 0.68       |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 19                  | 0.63     | 0.17                | 0.68       |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 19                  | 0.63     | 0.17                | 0.68       |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 19                  | 0.63     | 0.17                | 0.68       |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 19                  | 0.63     | 0.17                | 0.68       |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 19                  | 0.63     | 0.17                | 0.68       |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 19                  | 0.25     | 0.06                | 0.26       |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 18                  | 0.19     | 0.04                | 0.18       |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 18                  | 0.19     | 0.04                | 0.18       |
| (1,2)   | 1:37:A:TYR:HD1  | 1:57:A:ALA:HA   | 17                  | 0.21     | 0.07                | 0.2        |
| (1,2)   | 1:37:A:TYR:HD2  | 1:57:A:ALA:HA   | 17                  | 0.21     | 0.07                | 0.2        |
| (1,104) | 1:13:A:ALA:HA   | 1:14:A:GLU:H    | 17                  | 0.12     | 0.01                | 0.12       |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 16                  | 0.2      | 0.06                | 0.19       |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 16                  | 0.16     | 0.03                | 0.15       |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 16                  | 0.16     | 0.03                | 0.15       |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 15                  | 0.74     | 0.07                | 0.72       |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 14                  | 0.63     | 0.37                | 0.54       |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 14                  | 0.63     | 0.37                | 0.54       |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 14                  | 0.63     | 0.37                | 0.54       |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 14                  | 0.63     | 0.37                | 0.54       |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 14                  | 0.63     | 0.37                | 0.54       |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 14                  | 0.63     | 0.37                | 0.54       |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 14                  | 0.46     | 0.25                | 0.63       |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 13                  | 0.38     | 0.11                | 0.41       |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 13                  | 0.35     | 0.17                | 0.36       |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 13                  | 0.17     | 0.04                | 0.18       |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 13                  | 0.17     | 0.04                | 0.18       |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 12                  | 0.22     | 0.06                | 0.2        |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 12                  | 0.22     | 0.06                | 0.2        |
| (1,112) | 1:19:A:GLU:HA   | 1:20:A:THR:H    | 11                  | 0.19     | 0.03                | 0.19       |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 10                  | 0.92     | 0.49                | 0.82       |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 10                  | 0.92     | 0.49                | 0.82       |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 10                  | 0.92     | 0.49                | 0.82       |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 10                  | 0.92     | 0.49                | 0.82       |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 10                  | 0.92     | 0.49                | 0.82       |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 10                  | 0.92     | 0.49                | 0.82       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB1  | 9                   | 0.14     | 0.03                | 0.12       |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB2  | 9                   | 0.14     | 0.03                | 0.12       |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB3  | 9                   | 0.14     | 0.03                | 0.12       |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 8                   | 0.29     | 0.13                | 0.24       |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 8                   | 0.29     | 0.13                | 0.24       |
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 8                   | 0.29     | 0.13                | 0.24       |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 8                   | 0.16     | 0.07                | 0.12       |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 8                   | 0.16     | 0.07                | 0.12       |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 8                   | 0.16     | 0.07                | 0.12       |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 8                   | 0.16     | 0.07                | 0.12       |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 8                   | 0.16     | 0.07                | 0.12       |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 8                   | 0.16     | 0.07                | 0.12       |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB2  | 7                   | 1.27     | 1.27                | 0.53       |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB3  | 7                   | 1.27     | 1.27                | 0.53       |
| (1,205) | 1:38:A:CYS:HB2  | 1:48:A:TYR:H    | 7                   | 0.18     | 0.04                | 0.2        |
| (1,205) | 1:38:A:CYS:HB3  | 1:48:A:TYR:H    | 7                   | 0.18     | 0.04                | 0.2        |
| (1,218) | 1:50:A:THR:HA   | 1:52:A:ALA:H    | 5                   | 0.14     | 0.04                | 0.12       |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD11 | 4                   | 0.31     | 0.23                | 0.2        |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD12 | 4                   | 0.31     | 0.23                | 0.2        |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD13 | 4                   | 0.31     | 0.23                | 0.2        |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD21 | 4                   | 0.31     | 0.23                | 0.2        |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD22 | 4                   | 0.31     | 0.23                | 0.2        |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD23 | 4                   | 0.31     | 0.23                | 0.2        |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD11 | 4                   | 0.26     | 0.15                | 0.22       |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD12 | 4                   | 0.26     | 0.15                | 0.22       |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD13 | 4                   | 0.26     | 0.15                | 0.22       |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD11 | 4                   | 0.2      | 0.03                | 0.2        |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD12 | 4                   | 0.2      | 0.03                | 0.2        |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD13 | 4                   | 0.2      | 0.03                | 0.2        |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD11 | 4                   | 0.2      | 0.03                | 0.2        |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD12 | 4                   | 0.2      | 0.03                | 0.2        |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD13 | 4                   | 0.2      | 0.03                | 0.2        |
| (1,143) | 1:28:A:LEU:H    | 1:28:A:LEU:HB2  | 4                   | 0.14     | 0.03                | 0.14       |
| (1,143) | 1:28:A:LEU:H    | 1:28:A:LEU:HB3  | 4                   | 0.14     | 0.03                | 0.14       |
| (1,50)  | 1:55:A:ARG:HB2  | 1:56:A:HIS:HB2  | 3                   | 0.38     | 0.01                | 0.37       |
| (1,50)  | 1:55:A:ARG:HB2  | 1:56:A:HIS:HB3  | 3                   | 0.38     | 0.01                | 0.37       |
| (1,50)  | 1:55:A:ARG:HB3  | 1:56:A:HIS:HB2  | 3                   | 0.38     | 0.01                | 0.37       |
| (1,50)  | 1:55:A:ARG:HB3  | 1:56:A:HIS:HB3  | 3                   | 0.38     | 0.01                | 0.37       |
| (1,111) | 1:17:A:VAL:H    | 1:17:A:VAL:HB   | 3                   | 0.21     | 0.03                | 0.23       |
| (1,311) | 1:53:A:GLU:HG2  | 1:56:A:HIS:H    | 3                   | 0.15     | 0.02                | 0.15       |
| (1,311) | 1:53:A:GLU:HG3  | 1:56:A:HIS:H    | 3                   | 0.15     | 0.02                | 0.15       |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD11 | 2                   | 0.29     | 0.08                | 0.29       |

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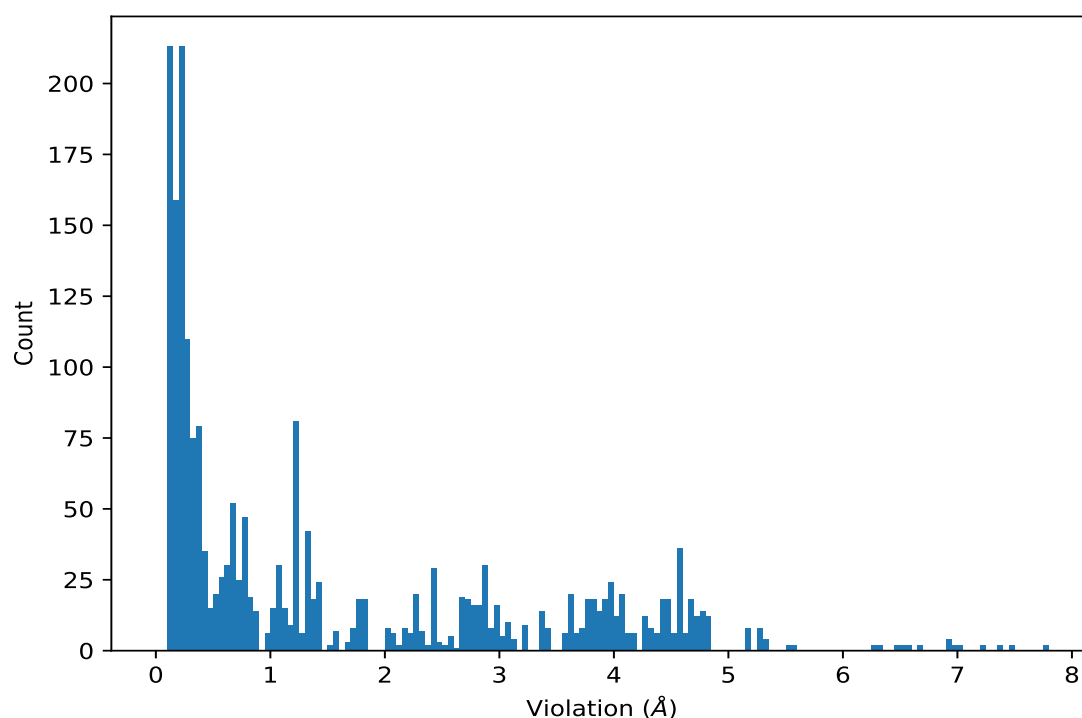
| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD12 | 2                   | 0.29     | 0.08                | 0.29       |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD13 | 2                   | 0.29     | 0.08                | 0.29       |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD21 | 2                   | 0.29     | 0.08                | 0.29       |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD22 | 2                   | 0.29     | 0.08                | 0.29       |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD23 | 2                   | 0.29     | 0.08                | 0.29       |
| (1,19)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HB2  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,19)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HB3  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,19)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HB2  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,19)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HB3  | 2                   | 0.22     | 0.01                | 0.22       |
| (1,348) | 1:11:A:LEU:HD11 | 1:12:A:SER:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,348) | 1:11:A:LEU:HD12 | 1:12:A:SER:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,348) | 1:11:A:LEU:HD13 | 1:12:A:SER:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,348) | 1:11:A:LEU:HD21 | 1:12:A:SER:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,348) | 1:11:A:LEU:HD22 | 1:12:A:SER:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,348) | 1:11:A:LEU:HD23 | 1:12:A:SER:H    | 2                   | 0.16     | 0.01                | 0.16       |
| (1,95)  | 1:11:A:LEU:H    | 1:11:A:LEU:HG   | 2                   | 0.16     | 0.02                | 0.16       |
| (1,42)  | 1:13:A:ALA:HB1  | 1:15:A:GLU:HA   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,42)  | 1:13:A:ALA:HB2  | 1:15:A:GLU:HA   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,42)  | 1:13:A:ALA:HB3  | 1:15:A:GLU:HA   | 2                   | 0.15     | 0.0                 | 0.15       |
| (1,295) | 1:13:A:ALA:H    | 1:14:A:GLU:H    | 2                   | 0.14     | 0.02                | 0.14       |
| (1,90)  | 1:6:A:GLY:H     | 1:7:A:ALA:H     | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key    | Atom-1         | Atom-2        | Model ID | Violation (Å) |
|--------|----------------|---------------|----------|---------------|
| (1,37) | 1:59:A:LEU:HB2 | 1:63:A:THR:HB | 19       | 7.77          |
| (1,37) | 1:59:A:LEU:HB3 | 1:63:A:THR:HB | 19       | 7.77          |
| (1,37) | 1:59:A:LEU:HB2 | 1:63:A:THR:HB | 8        | 7.49          |
| (1,37) | 1:59:A:LEU:HB3 | 1:63:A:THR:HB | 8        | 7.49          |
| (1,37) | 1:59:A:LEU:HB2 | 1:63:A:THR:HB | 12       | 7.39          |
| (1,37) | 1:59:A:LEU:HB3 | 1:63:A:THR:HB | 12       | 7.39          |
| (1,37) | 1:59:A:LEU:HB2 | 1:63:A:THR:HB | 15       | 7.21          |
| (1,37) | 1:59:A:LEU:HB3 | 1:63:A:THR:HB | 15       | 7.21          |
| (1,37) | 1:59:A:LEU:HB2 | 1:63:A:THR:HB | 6        | 7.0           |
| (1,37) | 1:59:A:LEU:HB3 | 1:63:A:THR:HB | 6        | 7.0           |
| (1,37) | 1:59:A:LEU:HB2 | 1:63:A:THR:HB | 18       | 6.95          |
| (1,37) | 1:59:A:LEU:HB3 | 1:63:A:THR:HB | 18       | 6.95          |
| (1,37) | 1:59:A:LEU:HB2 | 1:63:A:THR:HB | 7        | 6.93          |
| (1,37) | 1:59:A:LEU:HB3 | 1:63:A:THR:HB | 7        | 6.93          |
| (1,37) | 1:59:A:LEU:HB2 | 1:63:A:THR:HB | 13       | 6.93          |
| (1,37) | 1:59:A:LEU:HB3 | 1:63:A:THR:HB | 13       | 6.93          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 4        | 6.67          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 4        | 6.67          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 9        | 6.57          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 9        | 6.57          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 14       | 6.52          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 14       | 6.52          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 5        | 6.45          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 5        | 6.45          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 11       | 6.34          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 11       | 6.34          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 17       | 6.28          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 17       | 6.28          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 3        | 5.56          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 3        | 5.56          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 18       | 5.5           |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 18       | 5.5           |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 12       | 5.32          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 12       | 5.32          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 15       | 5.31          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 15       | 5.31          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 12       | 5.29          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 12       | 5.29          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 12       | 5.29          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 12       | 5.29          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 12       | 5.29          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 12       | 5.29          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 20       | 5.26          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 20       | 5.26          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB   | 2        | 5.18          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB   | 2        | 5.18          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 18       | 5.16          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 18       | 5.16          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 18       | 5.16          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 18       | 5.16          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 18       | 5.16          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 18       | 5.16          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 7        | 4.82          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 7        | 4.82          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 7        | 4.82          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 7        | 4.82          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 7        | 4.82          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 7        | 4.82          |

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| Key    | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|--------|----------------|-----------------|----------|---------------|
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD21 | 17       | 4.8           |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD22 | 17       | 4.8           |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD23 | 17       | 4.8           |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD21 | 17       | 4.8           |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD22 | 17       | 4.8           |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD23 | 17       | 4.8           |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD21 | 14       | 4.78          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD22 | 14       | 4.78          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD23 | 14       | 4.78          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD21 | 14       | 4.78          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD22 | 14       | 4.78          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD23 | 14       | 4.78          |
| (1,55) | 1:28:A:LEU:HG  | 1:38:A:CYS:HB2  | 1        | 4.75          |
| (1,55) | 1:28:A:LEU:HG  | 1:38:A:CYS:HB3  | 1        | 4.75          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD21 | 15       | 4.75          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD22 | 15       | 4.75          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD23 | 15       | 4.75          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD21 | 15       | 4.75          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD22 | 15       | 4.75          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD23 | 15       | 4.75          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD21 | 19       | 4.73          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD22 | 19       | 4.73          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD23 | 19       | 4.73          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD21 | 19       | 4.73          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD22 | 19       | 4.73          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD23 | 19       | 4.73          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD21 | 3        | 4.72          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD22 | 3        | 4.72          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD23 | 3        | 4.72          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD21 | 3        | 4.72          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD22 | 3        | 4.72          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD23 | 3        | 4.72          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD21 | 12       | 4.68          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD22 | 12       | 4.68          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD23 | 12       | 4.68          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD21 | 12       | 4.68          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD22 | 12       | 4.68          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD23 | 12       | 4.68          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD21 | 1        | 4.67          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD22 | 1        | 4.67          |
| (1,11) | 1:37:A:TYR:HE1 | 1:51:A:LEU:HD23 | 1        | 4.67          |
| (1,11) | 1:37:A:TYR:HE2 | 1:51:A:LEU:HD21 | 1        | 4.67          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 1        | 4.67          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 1        | 4.67          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 20       | 4.66          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 20       | 4.66          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 20       | 4.66          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 20       | 4.66          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 20       | 4.66          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 20       | 4.66          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 9        | 4.61          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 9        | 4.61          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 9        | 4.61          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 9        | 4.61          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 9        | 4.61          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 9        | 4.61          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 4        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 4        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 4        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 4        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 4        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 4        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 5        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 5        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 5        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 5        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 5        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 5        | 4.58          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 6        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 6        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 6        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 6        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 6        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 6        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 8        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 8        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 8        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 8        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 8        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 8        | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 13       | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 13       | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 13       | 4.57          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 13       | 4.57          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 13       | 4.57          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 13       | 4.57          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 16       | 4.55          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 16       | 4.55          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 16       | 4.55          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 16       | 4.55          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 16       | 4.55          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 16       | 4.55          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 18       | 4.53          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 18       | 4.53          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 18       | 4.53          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 18       | 4.53          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 18       | 4.53          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 18       | 4.53          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 2        | 4.49          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 2        | 4.49          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 2        | 4.49          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 2        | 4.49          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 2        | 4.49          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 2        | 4.49          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 4        | 4.47          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 4        | 4.47          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 4        | 4.47          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 4        | 4.47          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 4        | 4.47          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 4        | 4.47          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 10       | 4.45          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 10       | 4.45          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 10       | 4.45          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 10       | 4.45          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 10       | 4.45          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 10       | 4.45          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 15       | 4.44          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 15       | 4.44          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 15       | 4.44          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 15       | 4.44          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 15       | 4.44          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 15       | 4.44          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 14       | 4.42          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 14       | 4.42          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 14       | 4.42          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 14       | 4.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 14       | 4.42          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 14       | 4.42          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 20       | 4.42          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 20       | 4.42          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 20       | 4.42          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 20       | 4.42          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 20       | 4.42          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 20       | 4.42          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD21 | 11       | 4.37          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD22 | 11       | 4.37          |
| (1,11)  | 1:37:A:TYR:HE1  | 1:51:A:LEU:HD23 | 11       | 4.37          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD21 | 11       | 4.37          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD22 | 11       | 4.37          |
| (1,11)  | 1:37:A:TYR:HE2  | 1:51:A:LEU:HD23 | 11       | 4.37          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 7        | 4.32          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 7        | 4.32          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 7        | 4.32          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 7        | 4.32          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 7        | 4.32          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 7        | 4.32          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 4        | 4.3           |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 4        | 4.3           |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 2        | 4.28          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 2        | 4.28          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 2        | 4.28          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 2        | 4.28          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 2        | 4.28          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 2        | 4.28          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 10       | 4.28          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 10       | 4.28          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 10       | 4.28          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 10       | 4.28          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 10       | 4.28          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 10       | 4.28          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 12       | 4.16          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 12       | 4.16          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 12       | 4.16          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 12       | 4.16          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 12       | 4.16          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 12       | 4.16          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 3        | 4.1           |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 3        | 4.1           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 3        | 4.1           |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 3        | 4.1           |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 3        | 4.1           |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 3        | 4.1           |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 1        | 4.09          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 1        | 4.09          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 1        | 4.09          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 1        | 4.09          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 1        | 4.09          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 1        | 4.09          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 14       | 4.07          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 14       | 4.07          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 2        | 4.06          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 2        | 4.06          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 2        | 4.06          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 2        | 4.06          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 2        | 4.06          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 2        | 4.06          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 18       | 4.05          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 18       | 4.05          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 18       | 4.05          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 18       | 4.05          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 18       | 4.05          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 18       | 4.05          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 5        | 4.04          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 5        | 4.04          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 5        | 4.04          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 5        | 4.04          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 5        | 4.04          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 5        | 4.04          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 15       | 4.04          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 15       | 4.04          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 15       | 4.04          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 15       | 4.04          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 15       | 4.04          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 15       | 4.04          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 9        | 3.99          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 9        | 3.99          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 9        | 3.99          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 9        | 3.99          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 9        | 3.99          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 9        | 3.99          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 8        | 3.96          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 8        | 3.96          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 8        | 3.96          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 8        | 3.96          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 8        | 3.96          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 8        | 3.96          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 16       | 3.95          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 16       | 3.95          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 16       | 3.95          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 16       | 3.95          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 16       | 3.95          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 16       | 3.95          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 17       | 3.95          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 17       | 3.95          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 17       | 3.95          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 17       | 3.95          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 17       | 3.95          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 17       | 3.95          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 4        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 4        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 4        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 4        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 4        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 4        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 5        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 5        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 5        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 5        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 5        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 5        | 3.93          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 19       | 3.92          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 19       | 3.92          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 19       | 3.92          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 19       | 3.92          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 19       | 3.92          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 19       | 3.92          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 13       | 3.88          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 13       | 3.88          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 13       | 3.88          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 13       | 3.88          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 13       | 3.88          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 13       | 3.88          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 2        | 3.86          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 2        | 3.86          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 6        | 3.85          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 6        | 3.85          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 6        | 3.85          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 6        | 3.85          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 6        | 3.85          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 6        | 3.85          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 1        | 3.81          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 1        | 3.81          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 1        | 3.81          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 1        | 3.81          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 1        | 3.81          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 1        | 3.81          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 13       | 3.81          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 13       | 3.81          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 13       | 3.81          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 13       | 3.81          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 13       | 3.81          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 13       | 3.81          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 6        | 3.8           |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 6        | 3.8           |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 6        | 3.8           |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 6        | 3.8           |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 6        | 3.8           |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 6        | 3.8           |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 17       | 3.79          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 17       | 3.79          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 17       | 3.79          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 17       | 3.79          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 17       | 3.79          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 17       | 3.79          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 20       | 3.77          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 20       | 3.77          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 20       | 3.77          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 20       | 3.77          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 20       | 3.77          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 20       | 3.77          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 19       | 3.75          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 19       | 3.75          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 19       | 3.75          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 19       | 3.75          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 19       | 3.75          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 19       | 3.75          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 16       | 3.74          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 16       | 3.74          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 16       | 3.74          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 16       | 3.74          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 16       | 3.74          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 16       | 3.74          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 7        | 3.72          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 7        | 3.72          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 5        | 3.69          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 5        | 3.69          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 9        | 3.69          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 9        | 3.69          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB2  | 2        | 3.69          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB3  | 2        | 3.69          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2  | 6        | 3.64          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3  | 6        | 3.64          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 7        | 3.63          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 7        | 3.63          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 7        | 3.63          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 7        | 3.63          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 7        | 3.63          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 7        | 3.63          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 9        | 3.62          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 9        | 3.62          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 9        | 3.62          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 9        | 3.62          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 9        | 3.62          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 9        | 3.62          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD21 | 11       | 3.62          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD22 | 11       | 3.62          |
| (1,12)  | 1:37:A:TYR:HD1  | 1:51:A:LEU:HD23 | 11       | 3.62          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD21 | 11       | 3.62          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD22 | 11       | 3.62          |
| (1,12)  | 1:37:A:TYR:HD2  | 1:51:A:LEU:HD23 | 11       | 3.62          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H    | 10       | 3.55          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H    | 10       | 3.55          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H    | 10       | 3.55          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H    | 10       | 3.55          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H    | 10       | 3.55          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H    | 10       | 3.55          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2 | 13       | 3.44          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3 | 13       | 3.44          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H   | 11       | 3.41          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H   | 11       | 3.41          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H   | 11       | 3.41          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H   | 11       | 3.41          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H   | 11       | 3.41          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H   | 11       | 3.41          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H   | 14       | 3.36          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H   | 14       | 3.36          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H   | 14       | 3.36          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H   | 14       | 3.36          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H   | 14       | 3.36          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H   | 14       | 3.36          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 18       | 3.36          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 18       | 3.36          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 18       | 3.36          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 18       | 3.36          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 18       | 3.36          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 18       | 3.36          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2 | 8        | 3.36          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3 | 8        | 3.36          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 12       | 3.24          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 12       | 3.24          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 12       | 3.24          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 12       | 3.24          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 12       | 3.24          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 12       | 3.24          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 14       | 3.21          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2 | 19       | 3.21          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3 | 19       | 3.21          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 17       | 3.13          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 17       | 3.13          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 7        | 3.12          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 7        | 3.12          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2 | 16       | 3.09          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3 | 16       | 3.09          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 20       | 3.07          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 20       | 3.07          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 20       | 3.07          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 20       | 3.07          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 20       | 3.07          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 20       | 3.07          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 14       | 3.05          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 14       | 3.05          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 4        | 3.04          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 19       | 3.03          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 19       | 3.03          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 15       | 3.02          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 15       | 3.02          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 3        | 2.99          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 3        | 2.99          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 12       | 2.98          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 12       | 2.98          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2 | 18       | 2.96          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3 | 18       | 2.96          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2 | 11       | 2.94          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3 | 11       | 2.94          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H   | 3        | 2.91          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H   | 3        | 2.91          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H   | 3        | 2.91          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H   | 3        | 2.91          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H   | 3        | 2.91          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H   | 3        | 2.91          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 1        | 2.89          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 1        | 2.89          |
| (1,369) | 1:28:A:LEU:HD11 | 1:48:A:TYR:H   | 8        | 2.88          |
| (1,369) | 1:28:A:LEU:HD12 | 1:48:A:TYR:H   | 8        | 2.88          |
| (1,369) | 1:28:A:LEU:HD13 | 1:48:A:TYR:H   | 8        | 2.88          |
| (1,369) | 1:28:A:LEU:HD21 | 1:48:A:TYR:H   | 8        | 2.88          |
| (1,369) | 1:28:A:LEU:HD22 | 1:48:A:TYR:H   | 8        | 2.88          |
| (1,369) | 1:28:A:LEU:HD23 | 1:48:A:TYR:H   | 8        | 2.88          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2 | 10       | 2.87          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3 | 10       | 2.87          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 9        | 2.87          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 9        | 2.87          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 4        | 2.86          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 4        | 2.86          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 4        | 2.86          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 4        | 2.86          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 4        | 2.86          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 4        | 2.86          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2 | 12       | 2.86          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3 | 12       | 2.86          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 5        | 2.84          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 5        | 2.84          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 4        | 2.83          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 4        | 2.83          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 6        | 2.83          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 6        | 2.83          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 15       | 2.81          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 15       | 2.81          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 15       | 2.81          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 15       | 2.81          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 15       | 2.81          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 15       | 2.81          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 8        | 2.8           |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 8        | 2.8           |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 13       | 2.8           |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 13       | 2.8           |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 1        | 2.79          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 1        | 2.79          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 1        | 2.79          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 1        | 2.79          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 1        | 2.79          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 1        | 2.79          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 2        | 2.79          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 2        | 2.79          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 2        | 2.79          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 2        | 2.79          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 2        | 2.79          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 2        | 2.79          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 16       | 2.78          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 16       | 2.78          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2 | 17       | 2.76          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3 | 17       | 2.76          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 16       | 2.72          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 16       | 2.72          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 16       | 2.72          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 16       | 2.72          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 16       | 2.72          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 16       | 2.72          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2 | 20       | 2.72          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3 | 20       | 2.72          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 2        | 2.69          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 2        | 2.69          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 5        | 2.68          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 18       | 2.68          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 18       | 2.68          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 9        | 2.67          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 9        | 2.67          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 9        | 2.67          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 9        | 2.67          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 9        | 2.67          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 9        | 2.67          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 10       | 2.66          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 10       | 2.66          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 14       | 2.65          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 14       | 2.65          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 14       | 2.65          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 14       | 2.65          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 14       | 2.65          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 14       | 2.65          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 6        | 2.62          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 16       | 2.58          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 20       | 2.58          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 20       | 2.58          |
| (1,4)   | 1:37:A:TYR:HE1  | 1:51:A:LEU:HA  | 11       | 2.56          |
| (1,4)   | 1:37:A:TYR:HE2  | 1:51:A:LEU:HA  | 11       | 2.56          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 9        | 2.53          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 13       | 2.52          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 2        | 2.49          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 11       | 2.46          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 19       | 2.46          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 8        | 2.42          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 8        | 2.42          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 8        | 2.42          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 8        | 2.42          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 8        | 2.42          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 8        | 2.42          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 13       | 2.42          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 13       | 2.42          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 13       | 2.42          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 13       | 2.42          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 13       | 2.42          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 13       | 2.42          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 7        | 2.42          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB  | 10       | 2.42          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB  | 10       | 2.42          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3 | 1        | 2.41          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2 | 1        | 2.41          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3 | 1        | 2.41          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB2 | 3        | 2.41          |
| (1,55)  | 1:28:A:LEU:HG   | 1:38:A:CYS:HB3 | 3        | 2.41          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB2 | 18       | 2.36          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB3 | 18       | 2.36          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 7        | 2.34          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 7        | 2.34          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 7        | 2.34          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 7        | 2.34          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 7        | 2.34          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 7        | 2.34          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 8        | 2.3           |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2 | 15       | 2.29          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3 | 15       | 2.29          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 10       | 2.29          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 19       | 2.27          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 19       | 2.27          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 19       | 2.27          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 19       | 2.27          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 19       | 2.27          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 19       | 2.27          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H   | 17       | 2.27          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 5        | 2.21          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 5        | 2.21          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 5        | 2.21          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 5        | 2.21          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 5        | 2.21          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 5        | 2.21          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 17       | 2.18          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 17       | 2.18          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 17       | 2.18          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 17       | 2.18          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 17       | 2.18          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 17       | 2.18          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB  | 1        | 2.15          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB  | 1        | 2.15          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB  | 16       | 2.14          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB  | 16       | 2.14          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 3        | 2.07          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 3        | 2.07          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 3        | 2.07          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 3        | 2.07          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 3        | 2.07          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 3        | 2.07          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 6        | 2.04          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 6        | 2.04          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 6        | 2.04          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 6        | 2.04          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 6        | 2.04          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 6        | 2.04          |
| (1,37)  | 1:59:A:LEU:HB2  | 1:63:A:THR:HB  | 20       | 2.02          |
| (1,37)  | 1:59:A:LEU:HB3  | 1:63:A:THR:HB  | 20       | 2.02          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H   | 11       | 1.84          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H   | 11       | 1.84          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H   | 11       | 1.84          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H   | 11       | 1.84          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H   | 11       | 1.84          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H   | 11       | 1.84          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3 | 4        | 1.84          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2 | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3 | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2 | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3 | 2        | 1.77          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 2        | 1.77          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 2        | 1.77          |
| (1,368) | 1:28:A:LEU:HD11 | 1:39:A:CYS:H    | 10       | 1.76          |
| (1,368) | 1:28:A:LEU:HD12 | 1:39:A:CYS:H    | 10       | 1.76          |
| (1,368) | 1:28:A:LEU:HD13 | 1:39:A:CYS:H    | 10       | 1.76          |
| (1,368) | 1:28:A:LEU:HD21 | 1:39:A:CYS:H    | 10       | 1.76          |
| (1,368) | 1:28:A:LEU:HD22 | 1:39:A:CYS:H    | 10       | 1.76          |
| (1,368) | 1:28:A:LEU:HD23 | 1:39:A:CYS:H    | 10       | 1.76          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 11       | 1.74          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 11       | 1.74          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 11       | 1.74          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 11       | 1.74          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 11       | 1.74          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 11       | 1.74          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB2  | 11       | 1.73          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB3  | 11       | 1.73          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H    | 12       | 1.66          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H    | 3        | 1.65          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H    | 20       | 1.65          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 1        | 1.57          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 1        | 1.57          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 1        | 1.57          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 1        | 1.57          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 1        | 1.57          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 1        | 1.57          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H    | 18       | 1.56          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H    | 15       | 1.53          |
| (1,142) | 1:28:A:LEU:H    | 1:38:A:CYS:H    | 1        | 1.5           |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 9        | 1.43          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 9        | 1.43          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 9        | 1.43          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 12       | 1.42          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 12       | 1.42          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 12       | 1.42          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 12       | 1.42          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 12       | 1.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 12       | 1.42          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 5        | 1.41          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 5        | 1.41          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 1        | 1.41          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 1        | 1.41          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 1        | 1.41          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 7        | 1.39          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 7        | 1.39          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 7        | 1.39          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 16       | 1.37          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 16       | 1.37          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 16       | 1.37          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 14       | 1.36          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 14       | 1.36          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 6        | 1.34          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 6        | 1.34          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 6        | 1.34          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 13       | 1.34          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 13       | 1.34          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 13       | 1.34          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 19       | 1.33          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 19       | 1.33          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 19       | 1.33          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 6        | 1.32          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 9        | 1.32          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 9        | 1.32          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 18       | 1.32          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 18       | 1.32          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 18       | 1.32          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 18       | 1.32          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 18       | 1.32          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 18       | 1.32          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 3        | 1.3           |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 3        | 1.3           |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 3        | 1.3           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 20       | 1.28          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 20       | 1.28          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 20       | 1.28          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 20       | 1.28          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 20       | 1.28          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 20       | 1.28          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 2        | 1.24          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 2        | 1.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 2        | 1.24          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 15       | 1.23          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 15       | 1.23          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 15       | 1.23          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 20       | 1.23          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 20       | 1.23          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 20       | 1.23          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 10       | 1.22          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 10       | 1.22          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 10       | 1.22          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 12       | 1.22          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 12       | 1.22          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 12       | 1.22          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 14       | 1.22          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 14       | 1.22          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 14       | 1.22          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 1        | 1.21          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 1        | 1.21          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 1        | 1.21          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 2        | 1.21          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 2        | 1.21          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 2        | 1.21          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 5        | 1.21          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 5        | 1.21          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 5        | 1.21          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 7        | 1.21          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 7        | 1.21          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 7        | 1.21          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 9        | 1.21          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 9        | 1.21          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 9        | 1.21          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 13       | 1.21          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 13       | 1.21          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 13       | 1.21          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 14       | 1.21          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 14       | 1.21          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 14       | 1.21          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 16       | 1.2           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 16       | 1.2           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 16       | 1.2           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 16       | 1.2           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 16       | 1.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 16       | 1.2           |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 13       | 1.2           |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 13       | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 4        | 1.2           |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 4        | 1.2           |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 4        | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 6        | 1.2           |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 6        | 1.2           |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 6        | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 8        | 1.2           |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 8        | 1.2           |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 8        | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 11       | 1.2           |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 11       | 1.2           |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 11       | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 16       | 1.2           |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 16       | 1.2           |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 16       | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 17       | 1.2           |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 17       | 1.2           |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 17       | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 18       | 1.2           |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 18       | 1.2           |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 18       | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 19       | 1.2           |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 19       | 1.2           |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 19       | 1.2           |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 3        | 1.19          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 3        | 1.19          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 3        | 1.19          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 20       | 1.19          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 20       | 1.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 20       | 1.19          |
| (1,308) | 1:51:A:LEU:HD21 | 1:53:A:GLU:H    | 15       | 1.18          |
| (1,308) | 1:51:A:LEU:HD22 | 1:53:A:GLU:H    | 15       | 1.18          |
| (1,308) | 1:51:A:LEU:HD23 | 1:53:A:GLU:H    | 15       | 1.18          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 4        | 1.13          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 4        | 1.13          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 4        | 1.13          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 19       | 1.11          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 16       | 1.09          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 16       | 1.09          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 11       | 1.09          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 11       | 1.09          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 11       | 1.09          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 7        | 1.08          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 7        | 1.08          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 7        | 1.08          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 12       | 1.05          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 12       | 1.05          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 12       | 1.05          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 5        | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 5        | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 5        | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 8        | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 8        | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 8        | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 17       | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 17       | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 17       | 1.04          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 10       | 1.03          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 10       | 1.03          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 10       | 1.03          |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG21 | 18       | 1.0           |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG22 | 18       | 1.0           |
| (1,171) | 1:43:A:GLY:H    | 1:44:A:THR:HG23 | 18       | 1.0           |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 20       | 0.96          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 20       | 0.96          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 20       | 0.96          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 20       | 0.96          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 20       | 0.96          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 20       | 0.96          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 2        | 0.88          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 19       | 0.87          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 2        | 0.86          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 2        | 0.86          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 2        | 0.86          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 2        | 0.86          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 2        | 0.86          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 2        | 0.86          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 4        | 0.86          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 4        | 0.86          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 4        | 0.86          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 4        | 0.86          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 4        | 0.86          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 4        | 0.86          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 4        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 4        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 4        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 4        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 4        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 4        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 5        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 5        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 5        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 5        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 5        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 5        | 0.84          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 6        | 0.83          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 6        | 0.83          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 6        | 0.83          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 6        | 0.83          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 6        | 0.83          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 6        | 0.83          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 3        | 0.81          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 18       | 0.79          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 18       | 0.79          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 18       | 0.79          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 18       | 0.79          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 18       | 0.79          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 18       | 0.79          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 10       | 0.79          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 10       | 0.79          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 10       | 0.79          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 10       | 0.79          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 10       | 0.79          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 10       | 0.79          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 17       | 0.78          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 17       | 0.78          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 17       | 0.78          |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 15       | 0.78          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 13       | 0.77          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 13       | 0.77          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 13       | 0.77          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 13       | 0.77          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 13       | 0.77          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 13       | 0.77          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 13       | 0.77          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 11       | 0.76          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 11       | 0.76          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 8        | 0.75          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 12       | 0.75          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 15       | 0.75          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 4        | 0.72          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 8        | 0.71          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 8        | 0.71          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 8        | 0.71          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 8        | 0.71          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 8        | 0.71          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 8        | 0.71          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 7        | 0.71          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 9        | 0.71          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 14       | 0.71          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD11 | 2        | 0.7           |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD12 | 2        | 0.7           |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD13 | 2        | 0.7           |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD21 | 2        | 0.7           |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD22 | 2        | 0.7           |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD23 | 2        | 0.7           |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 15       | 0.7           |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 15       | 0.7           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 15       | 0.7           |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 15       | 0.7           |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 15       | 0.7           |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 15       | 0.7           |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 5        | 0.7           |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 6        | 0.7           |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 18       | 0.7           |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 7        | 0.69          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 7        | 0.69          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 7        | 0.69          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 7        | 0.69          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 7        | 0.69          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 7        | 0.69          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 10       | 0.69          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 10       | 0.69          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 3        | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 3        | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 3        | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 3        | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 3        | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 3        | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 20       | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 20       | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 20       | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 20       | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 20       | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 20       | 0.68          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 2        | 0.68          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 15       | 0.68          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 19       | 0.67          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 19       | 0.67          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 19       | 0.67          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 19       | 0.67          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 19       | 0.67          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 19       | 0.67          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 8        | 0.67          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 12       | 0.67          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 12       | 0.66          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 12       | 0.66          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 12       | 0.66          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 12       | 0.66          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 12       | 0.66          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 12       | 0.66          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 15       | 0.65          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 15       | 0.65          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 15       | 0.65          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 15       | 0.65          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 15       | 0.65          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 15       | 0.65          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 13       | 0.64          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 16       | 0.64          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 16       | 0.63          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 16       | 0.63          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 16       | 0.63          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 16       | 0.63          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 16       | 0.63          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 16       | 0.63          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 1        | 0.63          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 6        | 0.63          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 10       | 0.63          |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 1        | 0.61          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 17       | 0.6           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 17       | 0.6           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 17       | 0.6           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 17       | 0.6           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 17       | 0.6           |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 17       | 0.6           |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 8        | 0.6           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 8        | 0.6           |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 8        | 0.6           |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 2        | 0.59          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 2        | 0.59          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 2        | 0.59          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 2        | 0.59          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 2        | 0.59          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 2        | 0.59          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 2        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 2        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 2        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 2        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 2        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 2        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 9        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 9        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 9        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 9        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 9        | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 9        | 0.58          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 19       | 0.58          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 16       | 0.57          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 16       | 0.57          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 16       | 0.57          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 16       | 0.57          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 16       | 0.57          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 16       | 0.57          |
| (1,326) | 1:61:A:LEU:H    | 1:62:A:ASN:H    | 17       | 0.56          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD11 | 15       | 0.53          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD12 | 15       | 0.53          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD13 | 15       | 0.53          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 15       | 0.53          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 15       | 0.53          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 15       | 0.53          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB2  | 1        | 0.53          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB3  | 1        | 0.53          |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 11       | 0.52          |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 11       | 0.52          |
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 11       | 0.52          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 17       | 0.5           |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 17       | 0.5           |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 17       | 0.5           |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 17       | 0.5           |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 17       | 0.5           |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 17       | 0.5           |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD11 | 14       | 0.5           |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD12 | 14       | 0.5           |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD13 | 14       | 0.5           |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 1        | 0.49          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 1        | 0.49          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 1        | 0.49          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 1        | 0.49          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 1        | 0.49          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 1        | 0.49          |
| (1,93)  | 1:17:A:VAL:HA   | 1:18:A:MET:H    | 11       | 0.49          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 1        | 0.48          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 16       | 0.48          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 10       | 0.47          |
| (1,2)   | 1:37:A:TYR:HD1  | 1:57:A:ALA:HA   | 18       | 0.46          |
| (1,2)   | 1:37:A:TYR:HD2  | 1:57:A:ALA:HA   | 18       | 0.46          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 9        | 0.45          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 9        | 0.45          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 9        | 0.45          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 14       | 0.43          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 14       | 0.43          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 14       | 0.43          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 14       | 0.43          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 14       | 0.43          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 14       | 0.43          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 5        | 0.43          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 5        | 0.43          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 5        | 0.43          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 5        | 0.43          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 5        | 0.43          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 5        | 0.43          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 4        | 0.43          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 15       | 0.43          |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 17       | 0.42          |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 17       | 0.42          |
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 17       | 0.42          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 1        | 0.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 1        | 0.42          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 1        | 0.42          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 9        | 0.41          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 9        | 0.41          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 9        | 0.41          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 9        | 0.41          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 9        | 0.41          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 9        | 0.41          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 20       | 0.41          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 7        | 0.41          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 7        | 0.41          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 7        | 0.41          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 16       | 0.41          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 16       | 0.41          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 16       | 0.41          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 18       | 0.4           |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 4        | 0.4           |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 18       | 0.39          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 18       | 0.39          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 18       | 0.39          |
| (1,50)  | 1:55:A:ARG:HB2  | 1:56:A:HIS:HB2  | 18       | 0.39          |
| (1,50)  | 1:55:A:ARG:HB2  | 1:56:A:HIS:HB3  | 18       | 0.39          |
| (1,50)  | 1:55:A:ARG:HB3  | 1:56:A:HIS:HB2  | 18       | 0.39          |
| (1,50)  | 1:55:A:ARG:HB3  | 1:56:A:HIS:HB3  | 18       | 0.39          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 3        | 0.38          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 3        | 0.38          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 3        | 0.38          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 6        | 0.38          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 6        | 0.38          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 6        | 0.38          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 19       | 0.38          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 19       | 0.38          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 19       | 0.38          |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 8        | 0.38          |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD11 | 15       | 0.37          |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD12 | 15       | 0.37          |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD13 | 15       | 0.37          |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD21 | 15       | 0.37          |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD22 | 15       | 0.37          |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD23 | 15       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 2        | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 2        | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 2        | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 5        | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 5        | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 5        | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 11       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 11       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 11       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 13       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 13       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 13       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 15       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 15       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 15       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 20       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 20       | 0.37          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 20       | 0.37          |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 19       | 0.37          |
| (1,50)  | 1:55:A:ARG:HB2  | 1:56:A:HIS:HB2  | 3        | 0.37          |
| (1,50)  | 1:55:A:ARG:HB2  | 1:56:A:HIS:HB3  | 3        | 0.37          |
| (1,50)  | 1:55:A:ARG:HB3  | 1:56:A:HIS:HB2  | 3        | 0.37          |
| (1,50)  | 1:55:A:ARG:HB3  | 1:56:A:HIS:HB3  | 3        | 0.37          |
| (1,50)  | 1:55:A:ARG:HB2  | 1:56:A:HIS:HB2  | 16       | 0.37          |
| (1,50)  | 1:55:A:ARG:HB2  | 1:56:A:HIS:HB3  | 16       | 0.37          |
| (1,50)  | 1:55:A:ARG:HB3  | 1:56:A:HIS:HB2  | 16       | 0.37          |
| (1,50)  | 1:55:A:ARG:HB3  | 1:56:A:HIS:HB3  | 16       | 0.37          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 2        | 0.37          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 2        | 0.37          |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 7        | 0.36          |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 7        | 0.36          |
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 7        | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 8        | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 8        | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 8        | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 10       | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 10       | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 10       | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 14       | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 14       | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 14       | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG21 | 17       | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG22 | 17       | 0.36          |
| (1,172) | 1:44:A:THR:H    | 1:44:A:THR:HG23 | 17       | 0.36          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,146) | 1:29:A:LEU:H   | 1:29:A:LEU:HG   | 6        | 0.36          |
| (1,146) | 1:29:A:LEU:H   | 1:29:A:LEU:HG   | 16       | 0.36          |
| (1,319) | 1:62:A:ASN:H   | 1:63:A:THR:HA   | 9        | 0.35          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 2        | 0.35          |
| (1,172) | 1:44:A:THR:H   | 1:44:A:THR:HG21 | 4        | 0.35          |
| (1,172) | 1:44:A:THR:H   | 1:44:A:THR:HG22 | 4        | 0.35          |
| (1,172) | 1:44:A:THR:H   | 1:44:A:THR:HG23 | 4        | 0.35          |
| (1,172) | 1:44:A:THR:H   | 1:44:A:THR:HG21 | 12       | 0.35          |
| (1,172) | 1:44:A:THR:H   | 1:44:A:THR:HG22 | 12       | 0.35          |
| (1,172) | 1:44:A:THR:H   | 1:44:A:THR:HG23 | 12       | 0.35          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 11       | 0.35          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 11       | 0.35          |
| (1,146) | 1:29:A:LEU:H   | 1:29:A:LEU:HG   | 18       | 0.34          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 4        | 0.34          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 4        | 0.34          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 14       | 0.34          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 14       | 0.34          |
| (1,306) | 1:37:A:TYR:H   | 1:37:A:TYR:HE1  | 17       | 0.33          |
| (1,306) | 1:37:A:TYR:H   | 1:37:A:TYR:HE2  | 17       | 0.33          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 10       | 0.33          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 12       | 0.33          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 12       | 0.33          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 13       | 0.33          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 13       | 0.33          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 17       | 0.33          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 17       | 0.33          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 18       | 0.33          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 18       | 0.33          |
| (1,319) | 1:62:A:ASN:H   | 1:63:A:THR:HA   | 3        | 0.32          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 11       | 0.32          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 14       | 0.32          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 2        | 0.32          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 2        | 0.32          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 3        | 0.32          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 3        | 0.32          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 6        | 0.32          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 6        | 0.32          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 10       | 0.32          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 10       | 0.32          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD11 | 10       | 0.31          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD12 | 10       | 0.31          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD13 | 10       | 0.31          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD21 | 10       | 0.31          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD22 | 10       | 0.31          |
| (1,388) | 1:57:A:ALA:HA   | 1:61:A:LEU:HD23 | 10       | 0.31          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 1        | 0.31          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 1        | 0.31          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 1        | 0.31          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 1        | 0.31          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 1        | 0.31          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 1        | 0.31          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 19       | 0.31          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 19       | 0.31          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 1        | 0.31          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 9        | 0.31          |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 12       | 0.31          |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 18       | 0.31          |
| (1,58)  | 1:21:A:ARG:HB2  | 1:39:A:CYS:HB3  | 5        | 0.31          |
| (1,58)  | 1:21:A:ARG:HB3  | 1:39:A:CYS:HB3  | 5        | 0.31          |
| (1,58)  | 1:21:A:ARG:HB2  | 1:39:A:CYS:HB3  | 7        | 0.31          |
| (1,58)  | 1:21:A:ARG:HB3  | 1:39:A:CYS:HB3  | 7        | 0.31          |
| (1,58)  | 1:21:A:ARG:HB2  | 1:39:A:CYS:HB3  | 8        | 0.31          |
| (1,58)  | 1:21:A:ARG:HB3  | 1:39:A:CYS:HB3  | 8        | 0.31          |
| (1,58)  | 1:21:A:ARG:HB2  | 1:39:A:CYS:HB3  | 9        | 0.31          |
| (1,58)  | 1:21:A:ARG:HB3  | 1:39:A:CYS:HB3  | 9        | 0.31          |
| (1,53)  | 1:39:A:CYS:HB3  | 1:40:A:ILE:HG21 | 17       | 0.31          |
| (1,53)  | 1:39:A:CYS:HB3  | 1:40:A:ILE:HG22 | 17       | 0.31          |
| (1,53)  | 1:39:A:CYS:HB3  | 1:40:A:ILE:HG23 | 17       | 0.31          |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 14       | 0.31          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 18       | 0.3           |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 18       | 0.3           |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 18       | 0.3           |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 18       | 0.3           |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 18       | 0.3           |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 18       | 0.3           |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 6        | 0.3           |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 6        | 0.3           |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 20       | 0.3           |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 4        | 0.3           |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 5        | 0.3           |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 7        | 0.3           |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 8        | 0.3           |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 13       | 0.3           |
| (1,221) | 1:51:A:LEU:HA   | 1:53:A:GLU:H    | 15       | 0.3           |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 17       | 0.3           |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 1        | 0.3           |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 1        | 0.3           |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H    | 5        | 0.29          |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H    | 6        | 0.29          |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H    | 10       | 0.29          |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H    | 13       | 0.29          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 1        | 0.29          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 3        | 0.29          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 6        | 0.29          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 9        | 0.29          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 20       | 0.29          |
| (1,40)  | 1:56:A:HIS:HA  | 1:59:A:LEU:HG   | 9        | 0.29          |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H    | 8        | 0.28          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 16       | 0.28          |
| (1,221) | 1:51:A:LEU:HA  | 1:53:A:GLU:H    | 19       | 0.28          |
| (1,7)   | 1:37:A:TYR:HE1 | 1:58:A:CYS:HB2  | 1        | 0.28          |
| (1,7)   | 1:37:A:TYR:HE2 | 1:58:A:CYS:HB2  | 1        | 0.28          |
| (1,7)   | 1:37:A:TYR:HE1 | 1:58:A:CYS:HB2  | 7        | 0.28          |
| (1,7)   | 1:37:A:TYR:HE2 | 1:58:A:CYS:HB2  | 7        | 0.28          |
| (1,7)   | 1:37:A:TYR:HE1 | 1:58:A:CYS:HB2  | 17       | 0.28          |
| (1,7)   | 1:37:A:TYR:HE2 | 1:58:A:CYS:HB2  | 17       | 0.28          |
| (1,7)   | 1:37:A:TYR:HE1 | 1:58:A:CYS:HB2  | 19       | 0.28          |
| (1,7)   | 1:37:A:TYR:HE2 | 1:58:A:CYS:HB2  | 19       | 0.28          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD11 | 19       | 0.27          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD12 | 19       | 0.27          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD13 | 19       | 0.27          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD21 | 19       | 0.27          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD22 | 19       | 0.27          |
| (1,388) | 1:57:A:ALA:HA  | 1:61:A:LEU:HD23 | 19       | 0.27          |
| (1,375) | 1:39:A:CYS:H   | 1:61:A:LEU:HD11 | 18       | 0.27          |
| (1,375) | 1:39:A:CYS:H   | 1:61:A:LEU:HD12 | 18       | 0.27          |
| (1,375) | 1:39:A:CYS:H   | 1:61:A:LEU:HD13 | 18       | 0.27          |
| (1,375) | 1:39:A:CYS:H   | 1:61:A:LEU:HD21 | 18       | 0.27          |
| (1,375) | 1:39:A:CYS:H   | 1:61:A:LEU:HD22 | 18       | 0.27          |
| (1,375) | 1:39:A:CYS:H   | 1:61:A:LEU:HD23 | 18       | 0.27          |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H    | 2        | 0.27          |
| (1,275) | 1:28:A:LEU:H   | 1:28:A:LEU:HD11 | 2        | 0.27          |
| (1,275) | 1:28:A:LEU:H   | 1:28:A:LEU:HD12 | 2        | 0.27          |
| (1,275) | 1:28:A:LEU:H   | 1:28:A:LEU:HD13 | 2        | 0.27          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 19       | 0.27          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 19       | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 16       | 0.27          |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 19       | 0.27          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 10       | 0.27          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 10       | 0.27          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 11       | 0.27          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 11       | 0.27          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 14       | 0.27          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 14       | 0.27          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 11       | 0.26          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 11       | 0.26          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 11       | 0.26          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 11       | 0.26          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 11       | 0.26          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 11       | 0.26          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 14       | 0.26          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 17       | 0.26          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 19       | 0.26          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 17       | 0.26          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 17       | 0.26          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 9        | 0.26          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 9        | 0.26          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 9        | 0.26          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 16       | 0.26          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 16       | 0.26          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 16       | 0.26          |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 18       | 0.26          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB2  | 20       | 0.26          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB3  | 20       | 0.26          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 4        | 0.26          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 4        | 0.26          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 9        | 0.26          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 9        | 0.26          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 18       | 0.26          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 18       | 0.26          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD11 | 11       | 0.25          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD12 | 11       | 0.25          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD13 | 11       | 0.25          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD21 | 11       | 0.25          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD22 | 11       | 0.25          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD23 | 11       | 0.25          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 6        | 0.25          |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 6        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 6        | 0.25          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 6        | 0.25          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 6        | 0.25          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 6        | 0.25          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 11       | 0.25          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 7        | 0.25          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 7        | 0.25          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 12       | 0.25          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 12       | 0.25          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 1        | 0.25          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 1        | 0.25          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 1        | 0.25          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 20       | 0.25          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 20       | 0.25          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 20       | 0.25          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 3        | 0.25          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 3        | 0.25          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 5        | 0.25          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 5        | 0.25          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 6        | 0.25          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 6        | 0.25          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 12       | 0.25          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 12       | 0.25          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 13       | 0.25          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 13       | 0.25          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 16       | 0.25          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 16       | 0.25          |
| (1,2)   | 1:37:A:TYR:HD1  | 1:57:A:ALA:HA   | 9        | 0.25          |
| (1,2)   | 1:37:A:TYR:HD2  | 1:57:A:ALA:HA   | 9        | 0.25          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB2  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD11 | 1:38:A:CYS:HB3  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB2  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD12 | 1:38:A:CYS:HB3  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB2  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD13 | 1:38:A:CYS:HB3  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB2  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD21 | 1:38:A:CYS:HB3  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB2  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD22 | 1:38:A:CYS:HB3  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB2  | 3        | 0.24          |
| (1,367) | 1:28:A:LEU:HD23 | 1:38:A:CYS:HB3  | 3        | 0.24          |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 19       | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 19       | 0.24          |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 19       | 0.24          |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 19       | 0.24          |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 19       | 0.24          |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 19       | 0.24          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 16       | 0.24          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 16       | 0.24          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 4        | 0.24          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 7        | 0.24          |
| (1,300) | 1:28:A:LEU:HA   | 1:29:A:LEU:H    | 16       | 0.24          |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 5        | 0.24          |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 5        | 0.24          |
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 5        | 0.24          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 9        | 0.24          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 9        | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 7        | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 7        | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 7        | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 10       | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 10       | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 10       | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 12       | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 12       | 0.24          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 12       | 0.24          |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 11       | 0.24          |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 13       | 0.24          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 8        | 0.24          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 8        | 0.24          |
| (1,7)   | 1:37:A:TYR:HE1  | 1:58:A:CYS:HB2  | 15       | 0.24          |
| (1,7)   | 1:37:A:TYR:HE2  | 1:58:A:CYS:HB2  | 15       | 0.24          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD11 | 11       | 0.23          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD12 | 11       | 0.23          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD13 | 11       | 0.23          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD21 | 11       | 0.23          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD22 | 11       | 0.23          |
| (1,375) | 1:39:A:CYS:H    | 1:61:A:LEU:HD23 | 11       | 0.23          |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 2        | 0.23          |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 9        | 0.23          |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 9        | 0.23          |
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 9        | 0.23          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 2        | 0.23          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 2        | 0.23          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 3        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 3        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 3        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 6        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 6        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 6        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 8        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 8        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 8        | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 13       | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 13       | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 13       | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 15       | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 15       | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 15       | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 17       | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 17       | 0.23          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 17       | 0.23          |
| (1,111) | 1:17:A:VAL:H   | 1:17:A:VAL:HB   | 16       | 0.23          |
| (1,111) | 1:17:A:VAL:H   | 1:17:A:VAL:HB   | 17       | 0.23          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3  | 20       | 0.23          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3  | 20       | 0.23          |
| (1,19)  | 1:37:A:TYR:HD1 | 1:61:A:LEU:HB2  | 11       | 0.23          |
| (1,19)  | 1:37:A:TYR:HD1 | 1:61:A:LEU:HB3  | 11       | 0.23          |
| (1,19)  | 1:37:A:TYR:HD2 | 1:61:A:LEU:HB2  | 11       | 0.23          |
| (1,19)  | 1:37:A:TYR:HD2 | 1:61:A:LEU:HB3  | 11       | 0.23          |
| (1,7)   | 1:37:A:TYR:HE1 | 1:58:A:CYS:HB2  | 20       | 0.23          |
| (1,7)   | 1:37:A:TYR:HE2 | 1:58:A:CYS:HB2  | 20       | 0.23          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA   | 1        | 0.23          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA   | 1        | 0.23          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA   | 12       | 0.23          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA   | 12       | 0.23          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA   | 14       | 0.23          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA   | 14       | 0.23          |
| (1,306) | 1:37:A:TYR:H   | 1:37:A:TYR:HE1  | 9        | 0.22          |
| (1,306) | 1:37:A:TYR:H   | 1:37:A:TYR:HE2  | 9        | 0.22          |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H    | 18       | 0.22          |
| (1,251) | 1:55:A:ARG:HB2 | 1:57:A:ALA:H    | 14       | 0.22          |
| (1,251) | 1:55:A:ARG:HB3 | 1:57:A:ALA:H    | 14       | 0.22          |
| (1,218) | 1:50:A:THR:HA  | 1:52:A:ALA:H    | 2        | 0.22          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 11       | 0.22          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 11       | 0.22          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 11       | 0.22          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 19       | 0.22          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 19       | 0.22          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 19       | 0.22          |
| (1,138) | 1:25:A:ARG:H   | 1:39:A:CYS:HB3  | 8        | 0.22          |
| (1,40)  | 1:56:A:HIS:HA  | 1:59:A:LEU:HG   | 4        | 0.22          |
| (1,40)  | 1:56:A:HIS:HA  | 1:59:A:LEU:HG   | 5        | 0.22          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB2  | 10       | 0.22          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB3  | 10       | 0.22          |
| (1,23)  | 1:39:A:CYS:HB2 | 1:48:A:TYR:HE1  | 13       | 0.22          |
| (1,23)  | 1:39:A:CYS:HB2 | 1:48:A:TYR:HE2  | 13       | 0.22          |
| (1,13)  | 1:37:A:TYR:HD1 | 1:61:A:LEU:HD11 | 10       | 0.22          |
| (1,13)  | 1:37:A:TYR:HD1 | 1:61:A:LEU:HD12 | 10       | 0.22          |
| (1,13)  | 1:37:A:TYR:HD1 | 1:61:A:LEU:HD13 | 10       | 0.22          |
| (1,13)  | 1:37:A:TYR:HD2 | 1:61:A:LEU:HD11 | 10       | 0.22          |
| (1,13)  | 1:37:A:TYR:HD2 | 1:61:A:LEU:HD12 | 10       | 0.22          |
| (1,13)  | 1:37:A:TYR:HD2 | 1:61:A:LEU:HD13 | 10       | 0.22          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA   | 8        | 0.22          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA   | 8        | 0.22          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA   | 20       | 0.22          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA   | 20       | 0.22          |
| (1,319) | 1:62:A:ASN:H   | 1:63:A:THR:HA   | 6        | 0.21          |
| (1,306) | 1:37:A:TYR:H   | 1:37:A:TYR:HE1  | 5        | 0.21          |
| (1,306) | 1:37:A:TYR:H   | 1:37:A:TYR:HE2  | 5        | 0.21          |
| (1,294) | 1:15:A:GLU:H   | 1:16:A:GLY:H    | 6        | 0.21          |
| (1,251) | 1:55:A:ARG:HB2 | 1:57:A:ALA:H    | 19       | 0.21          |
| (1,251) | 1:55:A:ARG:HB3 | 1:57:A:ALA:H    | 19       | 0.21          |
| (1,205) | 1:38:A:CYS:HB2 | 1:48:A:TYR:H    | 7        | 0.21          |
| (1,205) | 1:38:A:CYS:HB3 | 1:48:A:TYR:H    | 7        | 0.21          |
| (1,205) | 1:38:A:CYS:HB2 | 1:48:A:TYR:H    | 17       | 0.21          |
| (1,205) | 1:38:A:CYS:HB3 | 1:48:A:TYR:H    | 17       | 0.21          |
| (1,205) | 1:38:A:CYS:HB2 | 1:48:A:TYR:H    | 18       | 0.21          |
| (1,205) | 1:38:A:CYS:HB3 | 1:48:A:TYR:H    | 18       | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 2        | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 2        | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 2        | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 4        | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 4        | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 4        | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG21 | 5        | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG22 | 5        | 0.21          |
| (1,169) | 1:42:A:GLY:H   | 1:44:A:THR:HG23 | 5        | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 18       | 0.21          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 18       | 0.21          |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 18       | 0.21          |
| (1,146) | 1:29:A:LEU:H    | 1:29:A:LEU:HG   | 5        | 0.21          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 10       | 0.21          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 13       | 0.21          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 20       | 0.21          |
| (1,112) | 1:19:A:GLU:HA   | 1:20:A:THR:H    | 16       | 0.21          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 4        | 0.21          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 4        | 0.21          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 5        | 0.21          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 5        | 0.21          |
| (1,19)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HB2  | 2        | 0.21          |
| (1,19)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HB3  | 2        | 0.21          |
| (1,19)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HB2  | 2        | 0.21          |
| (1,19)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HB3  | 2        | 0.21          |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD11 | 20       | 0.21          |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD12 | 20       | 0.21          |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD13 | 20       | 0.21          |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD11 | 20       | 0.21          |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD12 | 20       | 0.21          |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD13 | 20       | 0.21          |
| (1,2)   | 1:37:A:TYR:HD1  | 1:57:A:ALA:HA   | 7        | 0.21          |
| (1,2)   | 1:37:A:TYR:HD2  | 1:57:A:ALA:HA   | 7        | 0.21          |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD11 | 8        | 0.2           |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD12 | 8        | 0.2           |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD13 | 8        | 0.2           |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD21 | 8        | 0.2           |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD22 | 8        | 0.2           |
| (1,370) | 1:29:A:LEU:H    | 1:29:A:LEU:HD23 | 8        | 0.2           |
| (1,366) | 1:28:A:LEU:HD11 | 1:38:A:CYS:H    | 13       | 0.2           |
| (1,366) | 1:28:A:LEU:HD12 | 1:38:A:CYS:H    | 13       | 0.2           |
| (1,366) | 1:28:A:LEU:HD13 | 1:38:A:CYS:H    | 13       | 0.2           |
| (1,366) | 1:28:A:LEU:HD21 | 1:38:A:CYS:H    | 13       | 0.2           |
| (1,366) | 1:28:A:LEU:HD22 | 1:38:A:CYS:H    | 13       | 0.2           |
| (1,366) | 1:28:A:LEU:HD23 | 1:38:A:CYS:H    | 13       | 0.2           |
| (1,320) | 1:62:A:ASN:H    | 1:63:A:THR:HB   | 19       | 0.2           |
| (1,319) | 1:62:A:ASN:H    | 1:63:A:THR:HA   | 14       | 0.2           |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 11       | 0.2           |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 11       | 0.2           |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 14       | 0.2           |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 14       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 14       | 0.2           |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 18       | 0.2           |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 18       | 0.2           |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB1  | 7        | 0.2           |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB2  | 7        | 0.2           |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB3  | 7        | 0.2           |
| (1,205) | 1:38:A:CYS:HB2  | 1:48:A:TYR:H    | 10       | 0.2           |
| (1,205) | 1:38:A:CYS:HB3  | 1:48:A:TYR:H    | 10       | 0.2           |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG21 | 14       | 0.2           |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG22 | 14       | 0.2           |
| (1,169) | 1:42:A:GLY:H    | 1:44:A:THR:HG23 | 14       | 0.2           |
| (1,112) | 1:19:A:GLU:HA   | 1:20:A:THR:H    | 5        | 0.2           |
| (1,112) | 1:19:A:GLU:HA   | 1:20:A:THR:H    | 8        | 0.2           |
| (1,112) | 1:19:A:GLU:HA   | 1:20:A:THR:H    | 15       | 0.2           |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 1        | 0.2           |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 1        | 0.2           |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 2        | 0.2           |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 2        | 0.2           |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 15       | 0.2           |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 15       | 0.2           |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 18       | 0.2           |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 18       | 0.2           |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 20       | 0.2           |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 20       | 0.2           |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD11 | 16       | 0.2           |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD12 | 16       | 0.2           |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD13 | 16       | 0.2           |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD11 | 16       | 0.2           |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD12 | 16       | 0.2           |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD13 | 16       | 0.2           |
| (1,2)   | 1:37:A:TYR:HD1  | 1:57:A:ALA:HA   | 3        | 0.2           |
| (1,2)   | 1:37:A:TYR:HD2  | 1:57:A:ALA:HA   | 3        | 0.2           |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 4        | 0.19          |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 4        | 0.19          |
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 4        | 0.19          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 8        | 0.19          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 8        | 0.19          |
| (1,143) | 1:28:A:LEU:H    | 1:28:A:LEU:HB2  | 14       | 0.19          |
| (1,143) | 1:28:A:LEU:H    | 1:28:A:LEU:HB3  | 14       | 0.19          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 4        | 0.19          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 7        | 0.19          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 11       | 0.19          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,112) | 1:19:A:GLU:HA  | 1:20:A:THR:H   | 6        | 0.19          |
| (1,112) | 1:19:A:GLU:HA  | 1:20:A:THR:H   | 7        | 0.19          |
| (1,112) | 1:19:A:GLU:HA  | 1:20:A:THR:H   | 10       | 0.19          |
| (1,112) | 1:19:A:GLU:HA  | 1:20:A:THR:H   | 18       | 0.19          |
| (1,112) | 1:19:A:GLU:HA  | 1:20:A:THR:H   | 19       | 0.19          |
| (1,112) | 1:19:A:GLU:HA  | 1:20:A:THR:H   | 20       | 0.19          |
| (1,40)  | 1:56:A:HIS:HA  | 1:59:A:LEU:HG  | 8        | 0.19          |
| (1,40)  | 1:56:A:HIS:HA  | 1:59:A:LEU:HG  | 13       | 0.19          |
| (1,39)  | 1:57:A:ALA:HA  | 1:61:A:LEU:HB2 | 16       | 0.19          |
| (1,39)  | 1:57:A:ALA:HA  | 1:61:A:LEU:HB3 | 16       | 0.19          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA  | 4        | 0.19          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA  | 4        | 0.19          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA  | 5        | 0.19          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA  | 5        | 0.19          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA  | 13       | 0.19          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA  | 13       | 0.19          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA  | 16       | 0.19          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA  | 16       | 0.19          |
| (1,2)   | 1:37:A:TYR:HD1 | 1:57:A:ALA:HA  | 19       | 0.19          |
| (1,2)   | 1:37:A:TYR:HD2 | 1:57:A:ALA:HA  | 19       | 0.19          |
| (1,311) | 1:53:A:GLU:HG2 | 1:56:A:HIS:H   | 13       | 0.18          |
| (1,311) | 1:53:A:GLU:HG3 | 1:56:A:HIS:H   | 13       | 0.18          |
| (1,251) | 1:55:A:ARG:HB2 | 1:57:A:ALA:H   | 13       | 0.18          |
| (1,251) | 1:55:A:ARG:HB3 | 1:57:A:ALA:H   | 13       | 0.18          |
| (1,251) | 1:55:A:ARG:HB2 | 1:57:A:ALA:H   | 16       | 0.18          |
| (1,251) | 1:55:A:ARG:HB3 | 1:57:A:ALA:H   | 16       | 0.18          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB1 | 12       | 0.18          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB2 | 12       | 0.18          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB3 | 12       | 0.18          |
| (1,205) | 1:38:A:CYS:HB2 | 1:48:A:TYR:H   | 15       | 0.18          |
| (1,205) | 1:38:A:CYS:HB3 | 1:48:A:TYR:H   | 15       | 0.18          |
| (1,146) | 1:29:A:LEU:H   | 1:29:A:LEU:HG  | 9        | 0.18          |
| (1,138) | 1:25:A:ARG:H   | 1:39:A:CYS:HB3 | 3        | 0.18          |
| (1,138) | 1:25:A:ARG:H   | 1:39:A:CYS:HB3 | 12       | 0.18          |
| (1,138) | 1:25:A:ARG:H   | 1:39:A:CYS:HB3 | 17       | 0.18          |
| (1,58)  | 1:21:A:ARG:HB2 | 1:39:A:CYS:HB3 | 15       | 0.18          |
| (1,58)  | 1:21:A:ARG:HB3 | 1:39:A:CYS:HB3 | 15       | 0.18          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB2 | 14       | 0.18          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB3 | 14       | 0.18          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB2 | 18       | 0.18          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB3 | 18       | 0.18          |
| (1,23)  | 1:39:A:CYS:HB2 | 1:48:A:TYR:HE1 | 6        | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 6        | 0.18          |
| (1,348) | 1:11:A:LEU:HD11 | 1:12:A:SER:H    | 9        | 0.17          |
| (1,348) | 1:11:A:LEU:HD12 | 1:12:A:SER:H    | 9        | 0.17          |
| (1,348) | 1:11:A:LEU:HD13 | 1:12:A:SER:H    | 9        | 0.17          |
| (1,348) | 1:11:A:LEU:HD21 | 1:12:A:SER:H    | 9        | 0.17          |
| (1,348) | 1:11:A:LEU:HD22 | 1:12:A:SER:H    | 9        | 0.17          |
| (1,348) | 1:11:A:LEU:HD23 | 1:12:A:SER:H    | 9        | 0.17          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 4        | 0.17          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 4        | 0.17          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 13       | 0.17          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 13       | 0.17          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 5        | 0.17          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 5        | 0.17          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 15       | 0.17          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 15       | 0.17          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 2        | 0.17          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 2        | 0.17          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 2        | 0.17          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 10       | 0.17          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 10       | 0.17          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 10       | 0.17          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 6        | 0.17          |
| (1,95)  | 1:11:A:LEU:H    | 1:11:A:LEU:HG   | 4        | 0.17          |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 3        | 0.17          |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 6        | 0.17          |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 20       | 0.17          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 7        | 0.17          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 7        | 0.17          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 3        | 0.17          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 3        | 0.17          |
| (1,348) | 1:11:A:LEU:HD11 | 1:12:A:SER:H    | 12       | 0.16          |
| (1,348) | 1:11:A:LEU:HD12 | 1:12:A:SER:H    | 12       | 0.16          |
| (1,348) | 1:11:A:LEU:HD13 | 1:12:A:SER:H    | 12       | 0.16          |
| (1,348) | 1:11:A:LEU:HD21 | 1:12:A:SER:H    | 12       | 0.16          |
| (1,348) | 1:11:A:LEU:HD22 | 1:12:A:SER:H    | 12       | 0.16          |
| (1,348) | 1:11:A:LEU:HD23 | 1:12:A:SER:H    | 12       | 0.16          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 15       | 0.16          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 15       | 0.16          |
| (1,295) | 1:13:A:ALA:H    | 1:14:A:GLU:H    | 12       | 0.16          |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD11 | 13       | 0.16          |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD12 | 13       | 0.16          |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD13 | 13       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 4        | 0.16          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 4        | 0.16          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 11       | 0.16          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 11       | 0.16          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 11       | 0.16          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 14       | 0.16          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 14       | 0.16          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 14       | 0.16          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 5        | 0.16          |
| (1,111) | 1:17:A:VAL:H    | 1:17:A:VAL:HB   | 8        | 0.16          |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 7        | 0.16          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 12       | 0.16          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 12       | 0.16          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 11       | 0.16          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 11       | 0.16          |
| (1,2)   | 1:37:A:TYR:HD1  | 1:57:A:ALA:HA   | 15       | 0.16          |
| (1,2)   | 1:37:A:TYR:HD2  | 1:57:A:ALA:HA   | 15       | 0.16          |
| (1,2)   | 1:37:A:TYR:HD1  | 1:57:A:ALA:HA   | 17       | 0.16          |
| (1,2)   | 1:37:A:TYR:HD2  | 1:57:A:ALA:HA   | 17       | 0.16          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 10       | 0.15          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 10       | 0.15          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 10       | 0.15          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 10       | 0.15          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 10       | 0.15          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 10       | 0.15          |
| (1,317) | 1:58:A:CYS:H    | 1:59:A:LEU:HB2  | 2        | 0.15          |
| (1,317) | 1:58:A:CYS:H    | 1:59:A:LEU:HB3  | 2        | 0.15          |
| (1,311) | 1:53:A:GLU:HG2  | 1:56:A:HIS:H    | 18       | 0.15          |
| (1,311) | 1:53:A:GLU:HG3  | 1:56:A:HIS:H    | 18       | 0.15          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1  | 3        | 0.15          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2  | 3        | 0.15          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 1        | 0.15          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 1        | 0.15          |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB1  | 9        | 0.15          |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB2  | 9        | 0.15          |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB3  | 9        | 0.15          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 12       | 0.15          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 12       | 0.15          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 12       | 0.15          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 18       | 0.15          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 18       | 0.15          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 18       | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,143) | 1:28:A:LEU:H    | 1:28:A:LEU:HB2  | 2        | 0.15          |
| (1,143) | 1:28:A:LEU:H    | 1:28:A:LEU:HB3  | 2        | 0.15          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 14       | 0.15          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 18       | 0.15          |
| (1,81)  | 1:15:A:GLU:H    | 1:15:A:GLU:HB2  | 20       | 0.15          |
| (1,81)  | 1:15:A:GLU:H    | 1:15:A:GLU:HB3  | 20       | 0.15          |
| (1,58)  | 1:21:A:ARG:HB2  | 1:39:A:CYS:HB3  | 16       | 0.15          |
| (1,58)  | 1:21:A:ARG:HB3  | 1:39:A:CYS:HB3  | 16       | 0.15          |
| (1,42)  | 1:13:A:ALA:HB1  | 1:15:A:GLU:HA   | 12       | 0.15          |
| (1,42)  | 1:13:A:ALA:HB2  | 1:15:A:GLU:HA   | 12       | 0.15          |
| (1,42)  | 1:13:A:ALA:HB3  | 1:15:A:GLU:HA   | 12       | 0.15          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 11       | 0.15          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 11       | 0.15          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 13       | 0.15          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 13       | 0.15          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 17       | 0.15          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 17       | 0.15          |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD11 | 15       | 0.15          |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD12 | 15       | 0.15          |
| (1,13)  | 1:37:A:TYR:HD1  | 1:61:A:LEU:HD13 | 15       | 0.15          |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD11 | 15       | 0.15          |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD12 | 15       | 0.15          |
| (1,13)  | 1:37:A:TYR:HD2  | 1:61:A:LEU:HD13 | 15       | 0.15          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD11 | 1        | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD12 | 1        | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD13 | 1        | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD21 | 1        | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD22 | 1        | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD23 | 1        | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD11 | 10       | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD12 | 10       | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD13 | 10       | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD21 | 10       | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD22 | 10       | 0.14          |
| (1,390) | 1:58:A:CYS:H    | 1:61:A:LEU:HD23 | 10       | 0.14          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 11       | 0.14          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 18       | 0.14          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 3        | 0.14          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 3        | 0.14          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 3        | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 3        | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 3        | 0.14          |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H   | 4        | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H   | 4        | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H   | 4        | 0.14          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H   | 5        | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H   | 5        | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H   | 5        | 0.14          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H   | 6        | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H   | 6        | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H   | 6        | 0.14          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H   | 7        | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H   | 7        | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H   | 7        | 0.14          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H   | 8        | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H   | 8        | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H   | 8        | 0.14          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H   | 13       | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H   | 13       | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H   | 13       | 0.14          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H   | 15       | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H   | 15       | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H   | 15       | 0.14          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H   | 17       | 0.14          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H   | 17       | 0.14          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H   | 17       | 0.14          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3 | 16       | 0.14          |
| (1,95)  | 1:11:A:LEU:H    | 1:11:A:LEU:HG  | 8        | 0.14          |
| (1,42)  | 1:13:A:ALA:HB1  | 1:15:A:GLU:HA  | 20       | 0.14          |
| (1,42)  | 1:13:A:ALA:HB2  | 1:15:A:GLU:HA  | 20       | 0.14          |
| (1,42)  | 1:13:A:ALA:HB3  | 1:15:A:GLU:HA  | 20       | 0.14          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB2 | 17       | 0.14          |
| (1,39)  | 1:57:A:ALA:HA   | 1:61:A:LEU:HB3 | 17       | 0.14          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2 | 5        | 0.14          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3 | 5        | 0.14          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2 | 8        | 0.14          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3 | 8        | 0.14          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1 | 14       | 0.14          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2 | 14       | 0.14          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H   | 3        | 0.13          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE1 | 8        | 0.13          |
| (1,306) | 1:37:A:TYR:H    | 1:37:A:TYR:HE2 | 8        | 0.13          |
| (1,262) | 1:58:A:CYS:HB2  | 1:59:A:LEU:H   | 10       | 0.13          |
| (1,262) | 1:58:A:CYS:HB3  | 1:59:A:LEU:H   | 10       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 6        | 0.13          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 6        | 0.13          |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB1  | 5        | 0.13          |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB2  | 5        | 0.13          |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB3  | 5        | 0.13          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 1        | 0.13          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 1        | 0.13          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 1        | 0.13          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 9        | 0.13          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 9        | 0.13          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 9        | 0.13          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 16       | 0.13          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 16       | 0.13          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 16       | 0.13          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 19       | 0.13          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 19       | 0.13          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 19       | 0.13          |
| (1,226) | 1:51:A:LEU:HD11 | 1:53:A:GLU:H    | 20       | 0.13          |
| (1,226) | 1:51:A:LEU:HD12 | 1:53:A:GLU:H    | 20       | 0.13          |
| (1,226) | 1:51:A:LEU:HD13 | 1:53:A:GLU:H    | 20       | 0.13          |
| (1,218) | 1:50:A:THR:HA   | 1:52:A:ALA:H    | 12       | 0.13          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 2        | 0.13          |
| (1,138) | 1:25:A:ARG:H    | 1:39:A:CYS:HB3  | 9        | 0.13          |
| (1,104) | 1:13:A:ALA:HA   | 1:14:A:GLU:H    | 5        | 0.13          |
| (1,104) | 1:13:A:ALA:HA   | 1:14:A:GLU:H    | 10       | 0.13          |
| (1,104) | 1:13:A:ALA:HA   | 1:14:A:GLU:H    | 11       | 0.13          |
| (1,104) | 1:13:A:ALA:HA   | 1:14:A:GLU:H    | 13       | 0.13          |
| (1,40)  | 1:56:A:HIS:HA   | 1:59:A:LEU:HG   | 12       | 0.13          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 4        | 0.13          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 4        | 0.13          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 9        | 0.13          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 9        | 0.13          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB2  | 20       | 0.13          |
| (1,34)  | 1:51:A:LEU:HA   | 1:53:A:GLU:HB3  | 20       | 0.13          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE1  | 8        | 0.13          |
| (1,23)  | 1:39:A:CYS:HB2  | 1:48:A:TYR:HE2  | 8        | 0.13          |
| (1,2)   | 1:37:A:TYR:HD1  | 1:57:A:ALA:HA   | 6        | 0.13          |
| (1,2)   | 1:37:A:TYR:HD2  | 1:57:A:ALA:HA   | 6        | 0.13          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 1        | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 1        | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 1        | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 1        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 1        | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 1        | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 16       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 16       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 16       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 16       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 16       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 16       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 17       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 17       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 17       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 17       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 17       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 17       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 19       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 19       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 19       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 19       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 19       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 19       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD11 | 20       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD12 | 20       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD13 | 20       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD21 | 20       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD22 | 20       | 0.12          |
| (1,391) | 1:61:A:LEU:H    | 1:61:A:LEU:HD23 | 20       | 0.12          |
| (1,384) | 1:53:A:GLU:H    | 1:54:A:CYS:HB2  | 2        | 0.12          |
| (1,384) | 1:53:A:GLU:H    | 1:54:A:CYS:HB3  | 2        | 0.12          |
| (1,325) | 1:62:A:ASN:HA   | 1:63:A:THR:H    | 4        | 0.12          |
| (1,311) | 1:53:A:GLU:HG2  | 1:56:A:HIS:H    | 10       | 0.12          |
| (1,311) | 1:53:A:GLU:HG3  | 1:56:A:HIS:H    | 10       | 0.12          |
| (1,298) | 1:11:A:LEU:H    | 1:12:A:SER:H    | 4        | 0.12          |
| (1,295) | 1:13:A:ALA:H    | 1:14:A:GLU:H    | 20       | 0.12          |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD11 | 1        | 0.12          |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD12 | 1        | 0.12          |
| (1,275) | 1:28:A:LEU:H    | 1:28:A:LEU:HD13 | 1        | 0.12          |
| (1,270) | 1:61:A:LEU:HD11 | 1:62:A:ASN:H    | 6        | 0.12          |
| (1,270) | 1:61:A:LEU:HD12 | 1:62:A:ASN:H    | 6        | 0.12          |
| (1,270) | 1:61:A:LEU:HD13 | 1:62:A:ASN:H    | 6        | 0.12          |
| (1,251) | 1:55:A:ARG:HB2  | 1:57:A:ALA:H    | 11       | 0.12          |
| (1,251) | 1:55:A:ARG:HB3  | 1:57:A:ALA:H    | 11       | 0.12          |
| (1,248) | 1:56:A:HIS:H    | 1:57:A:ALA:HB1  | 13       | 0.12          |

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| Key     | Atom-1         | Atom-2         | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB2 | 13       | 0.12          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB3 | 13       | 0.12          |
| (1,237) | 1:55:A:ARG:H   | 1:57:A:ALA:HB1 | 17       | 0.12          |
| (1,237) | 1:55:A:ARG:H   | 1:57:A:ALA:HB2 | 17       | 0.12          |
| (1,237) | 1:55:A:ARG:H   | 1:57:A:ALA:HB3 | 17       | 0.12          |
| (1,218) | 1:50:A:THR:HA  | 1:52:A:ALA:H   | 10       | 0.12          |
| (1,218) | 1:50:A:THR:HA  | 1:52:A:ALA:H   | 17       | 0.12          |
| (1,205) | 1:38:A:CYS:HB2 | 1:48:A:TYR:H   | 12       | 0.12          |
| (1,205) | 1:38:A:CYS:HB3 | 1:48:A:TYR:H   | 12       | 0.12          |
| (1,205) | 1:38:A:CYS:HB2 | 1:48:A:TYR:H   | 14       | 0.12          |
| (1,205) | 1:38:A:CYS:HB3 | 1:48:A:TYR:H   | 14       | 0.12          |
| (1,143) | 1:28:A:LEU:H   | 1:28:A:LEU:HB2 | 13       | 0.12          |
| (1,143) | 1:28:A:LEU:H   | 1:28:A:LEU:HB3 | 13       | 0.12          |
| (1,138) | 1:25:A:ARG:H   | 1:39:A:CYS:HB3 | 1        | 0.12          |
| (1,138) | 1:25:A:ARG:H   | 1:39:A:CYS:HB3 | 15       | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 1        | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 2        | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 4        | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 7        | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 8        | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 15       | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 16       | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 17       | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 18       | 0.12          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H   | 19       | 0.12          |
| (1,40)  | 1:56:A:HIS:HA  | 1:59:A:LEU:HG  | 17       | 0.12          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB2 | 6        | 0.12          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB3 | 6        | 0.12          |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H   | 12       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB1 | 4        | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB2 | 4        | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB3 | 4        | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB1 | 14       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB2 | 14       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB3 | 14       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB1 | 17       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB2 | 17       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB3 | 17       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB1 | 19       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB2 | 19       | 0.11          |
| (1,248) | 1:56:A:HIS:H   | 1:57:A:ALA:HB3 | 19       | 0.11          |
| (1,218) | 1:50:A:THR:HA  | 1:52:A:ALA:H   | 15       | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,146) | 1:29:A:LEU:H   | 1:29:A:LEU:HG   | 10       | 0.11          |
| (1,138) | 1:25:A:ARG:H   | 1:39:A:CYS:HB3  | 19       | 0.11          |
| (1,112) | 1:19:A:GLU:HA  | 1:20:A:THR:H    | 17       | 0.11          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H    | 3        | 0.11          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H    | 6        | 0.11          |
| (1,104) | 1:13:A:ALA:HA  | 1:14:A:GLU:H    | 9        | 0.11          |
| (1,40)  | 1:56:A:HIS:HA  | 1:59:A:LEU:HG   | 15       | 0.11          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB2  | 15       | 0.11          |
| (1,34)  | 1:51:A:LEU:HA  | 1:53:A:GLU:HB3  | 15       | 0.11          |
| (1,325) | 1:62:A:ASN:HA  | 1:63:A:THR:H    | 14       | 0.1           |
| (1,300) | 1:28:A:LEU:HA  | 1:29:A:LEU:H    | 3        | 0.1           |
| (1,299) | 1:5:A:VAL:H    | 1:6:A:GLY:H     | 7        | 0.1           |
| (1,266) | 1:61:A:LEU:H   | 1:61:A:LEU:HD21 | 18       | 0.1           |
| (1,266) | 1:61:A:LEU:H   | 1:61:A:LEU:HD22 | 18       | 0.1           |
| (1,266) | 1:61:A:LEU:H   | 1:61:A:LEU:HD23 | 18       | 0.1           |
| (1,261) | 1:59:A:LEU:H   | 1:59:A:LEU:HB2  | 10       | 0.1           |
| (1,261) | 1:59:A:LEU:H   | 1:59:A:LEU:HB3  | 10       | 0.1           |
| (1,143) | 1:28:A:LEU:H   | 1:28:A:LEU:HB2  | 1        | 0.1           |
| (1,143) | 1:28:A:LEU:H   | 1:28:A:LEU:HB3  | 1        | 0.1           |
| (1,90)  | 1:6:A:GLY:H    | 1:7:A:ALA:H     | 8        | 0.1           |
| (1,90)  | 1:6:A:GLY:H    | 1:7:A:ALA:H     | 11       | 0.1           |
| (1,87)  | 1:5:A:VAL:HG11 | 1:6:A:GLY:H     | 6        | 0.1           |
| (1,87)  | 1:5:A:VAL:HG12 | 1:6:A:GLY:H     | 6        | 0.1           |
| (1,87)  | 1:5:A:VAL:HG13 | 1:6:A:GLY:H     | 6        | 0.1           |
| (1,23)  | 1:39:A:CYS:HB2 | 1:48:A:TYR:HE1  | 16       | 0.1           |
| (1,23)  | 1:39:A:CYS:HB2 | 1:48:A:TYR:HE2  | 16       | 0.1           |

## 10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found