



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:48 AM UTC

PDB ID : 2N0Z / pdb\_00002n0z  
BMRB ID : 25541  
Title : Solution structure of MyUb (1080-1122) of human Myosin VI  
Authors : He, F.; Walters, K.  
Deposited on : 2015-03-20

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

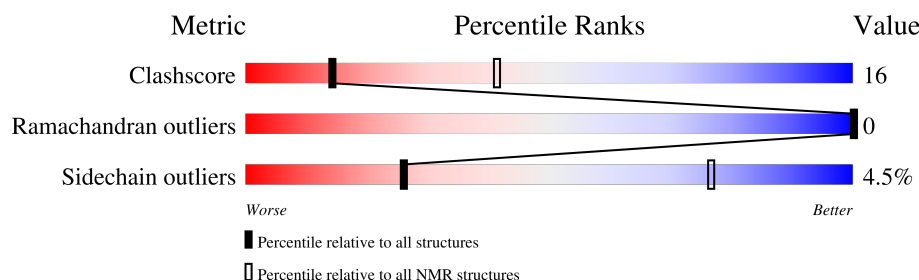
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 91%.

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     | 51     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                       |                   |              |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:14-A:46 (33)        | 0.30              | 10           |

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 and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 829 atoms, of which 413 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Unconventional myosin-VI.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 51       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 829   | 261 | 413 | 75 | 78 | 2 |       |

There are 8 discrepancies between the modelled and reference sequences:

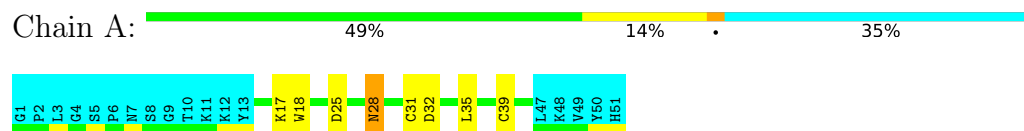
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | GLY      | -      | expression tag | UNP Q5JVM0 |
| A     | 2       | PRO      | -      | expression tag | UNP Q5JVM0 |
| A     | 3       | LEU      | -      | expression tag | UNP Q5JVM0 |
| A     | 4       | GLY      | -      | expression tag | UNP Q5JVM0 |
| A     | 5       | SER      | -      | expression tag | UNP Q5JVM0 |
| A     | 6       | PRO      | -      | expression tag | UNP Q5JVM0 |
| A     | 7       | ASN      | -      | expression tag | UNP Q5JVM0 |
| A     | 8       | SER      | -      | expression tag | UNP Q5JVM0 |

## 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: Unconventional myosin-VI

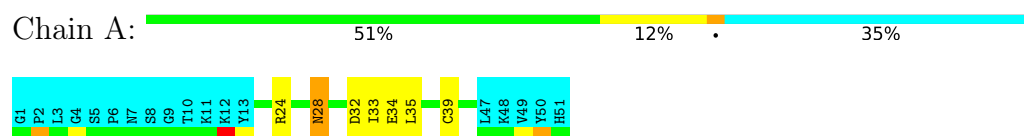


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

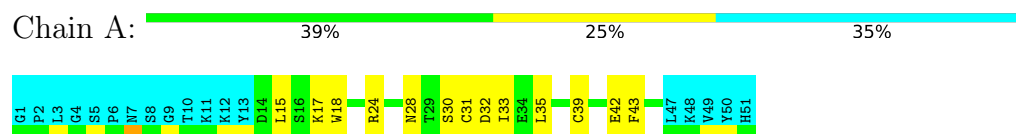
#### 4.2.1 Score per residue for model 1

- Molecule 1: Unconventional myosin-VI



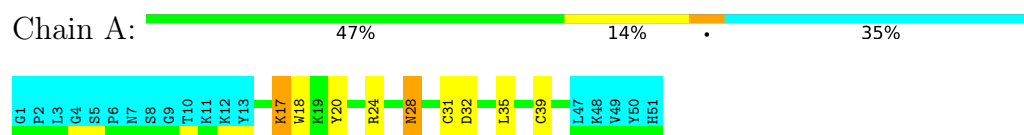
#### 4.2.2 Score per residue for model 2

- Molecule 1: Unconventional myosin-VI



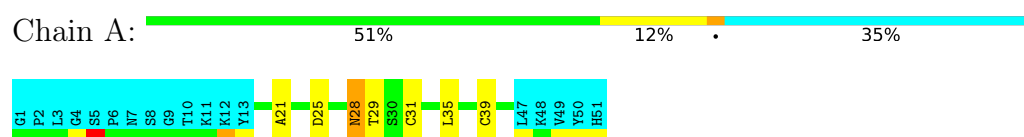
### 4.2.3 Score per residue for model 3

- Molecule 1: Unconventional myosin-VI



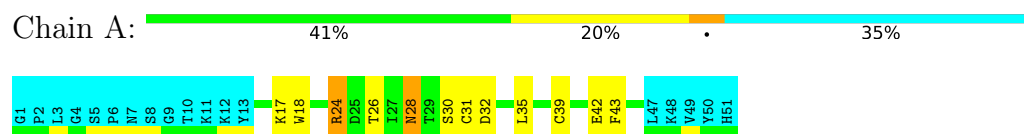
### 4.2.4 Score per residue for model 4

- Molecule 1: Unconventional myosin-VI



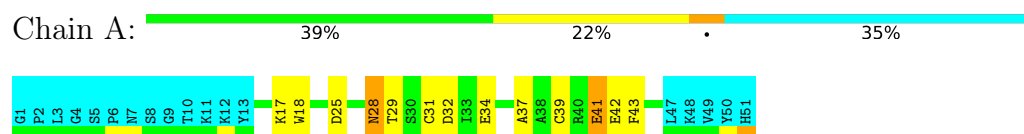
### 4.2.5 Score per residue for model 5

- Molecule 1: Unconventional myosin-VI



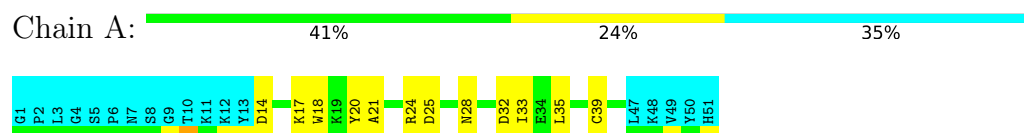
### 4.2.6 Score per residue for model 6

- Molecule 1: Unconventional myosin-VI



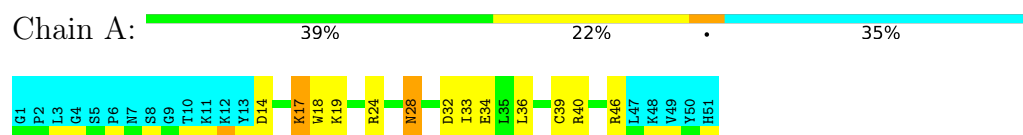
### 4.2.7 Score per residue for model 7

- Molecule 1: Unconventional myosin-VI



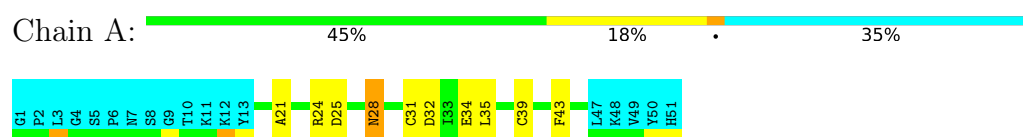
### 4.2.8 Score per residue for model 8

- Molecule 1: Unconventional myosin-VI



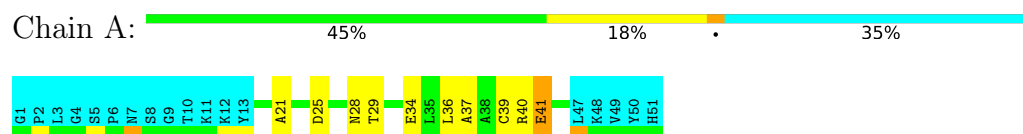
### 4.2.9 Score per residue for model 9

- Molecule 1: Unconventional myosin-VI



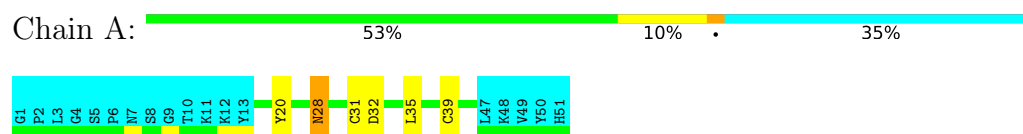
### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Unconventional myosin-VI



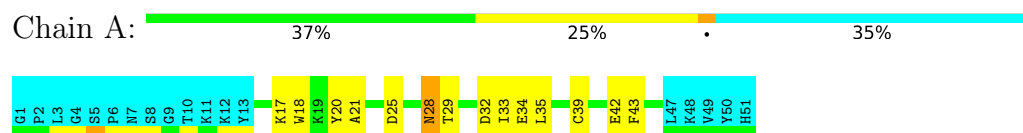
### 4.2.11 Score per residue for model 11

- Molecule 1: Unconventional myosin-VI



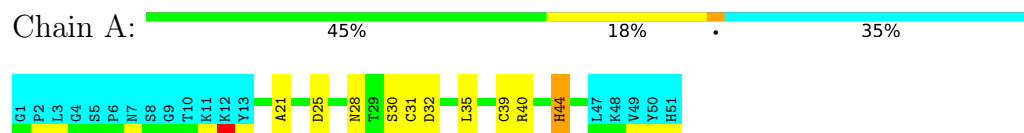
### 4.2.12 Score per residue for model 12

- Molecule 1: Unconventional myosin-VI



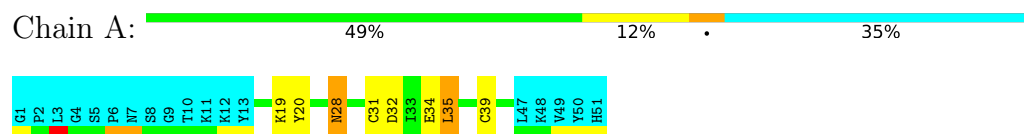
### 4.2.13 Score per residue for model 13

- Molecule 1: Unconventional myosin-VI



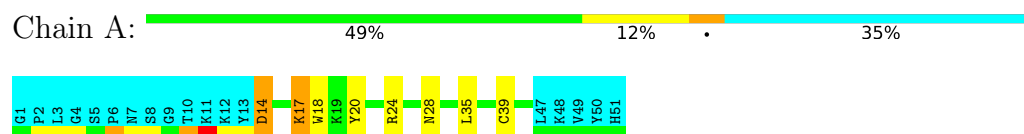
### 4.2.14 Score per residue for model 14

- Molecule 1: Unconventional myosin-VI



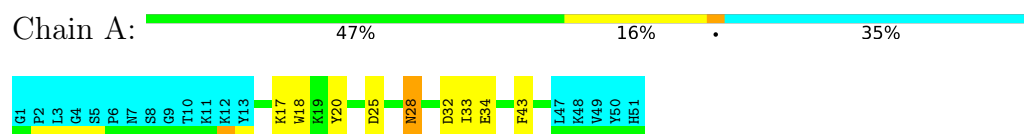
### 4.2.15 Score per residue for model 15

- Molecule 1: Unconventional myosin-VI



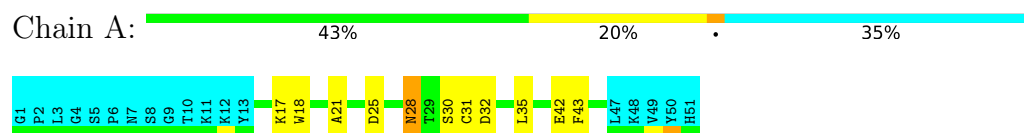
### 4.2.16 Score per residue for model 16

- Molecule 1: Unconventional myosin-VI



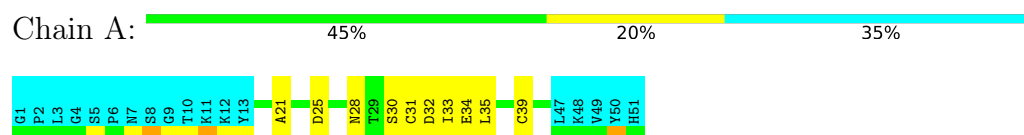
### 4.2.17 Score per residue for model 17

- Molecule 1: Unconventional myosin-VI



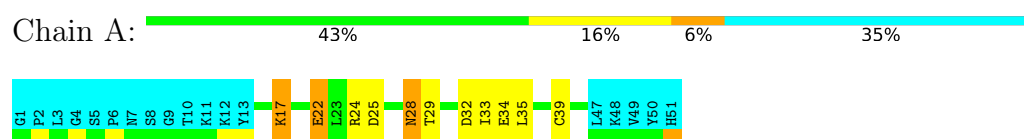
### 4.2.18 Score per residue for model 18

- Molecule 1: Unconventional myosin-VI



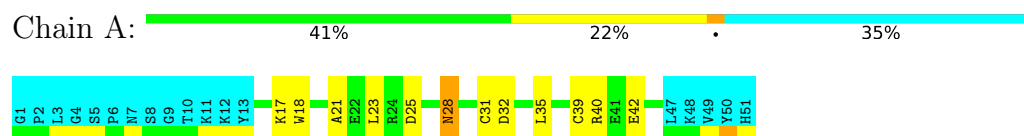
### 4.2.19 Score per residue for model 19

- Molecule 1: Unconventional myosin-VI



### 4.2.20 Score per residue for model 20

- Molecule 1: Unconventional myosin-VI



## 5 Refinement protocol and experimental data overview

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

Of the 98 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| X-PLOR NIH    | refinement            |         |
| CYANA         | structure calculation | 2.1     |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 651            |
| Number of shifts mapped to atoms             | 651            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 91%            |

## 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     | 278   | 270      | 270      | 8±2     |
| All | All   | 5560  | 5400     | 5400     | 170     |

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 16.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:28:ASN:HD22 | 1:A:28:ASN:N    | 0.59     | 1.96        | 4      | 17    |
| 1:A:39:CYS:SG   | 1:A:40:ARG:N    | 0.57     | 2.77        | 10     | 3     |
| 1:A:24:ARG:NH1  | 1:A:43:PHE:CE1  | 0.55     | 2.75        | 5      | 1     |
| 1:A:17:LYS:O    | 1:A:18:TRP:CD1  | 0.53     | 2.62        | 2      | 11    |
| 1:A:25:ASP:O    | 1:A:29:THR:N    | 0.53     | 2.42        | 6      | 2     |
| 1:A:19:LYS:N    | 1:A:19:LYS:CD   | 0.53     | 2.71        | 8      | 2     |
| 1:A:34:GLU:N    | 1:A:34:GLU:CD   | 0.53     | 2.67        | 10     | 2     |
| 1:A:41:GLU:OE1  | 1:A:41:GLU:N    | 0.53     | 2.42        | 6      | 1     |
| 1:A:22:GLU:N    | 1:A:22:GLU:OE1  | 0.52     | 2.43        | 19     | 1     |
| 1:A:44:HIS:N    | 1:A:44:HIS:ND1  | 0.52     | 2.56        | 13     | 1     |
| 1:A:24:ARG:NH1  | 1:A:43:PHE:CD1  | 0.51     | 2.78        | 5      | 1     |
| 1:A:24:ARG:O    | 1:A:28:ASN:ND2  | 0.51     | 2.42        | 15     | 7     |
| 1:A:35:LEU:O    | 1:A:39:CYS:SG   | 0.51     | 2.69        | 19     | 14    |
| 1:A:24:ARG:NH2  | 1:A:28:ASN:HD21 | 0.50     | 2.04        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:28:ASN:N    | 1:A:28:ASN:ND2  | 0.49     | 2.60        | 17     | 5     |
| 1:A:42:GLU:OE1  | 1:A:43:PHE:N    | 0.48     | 2.46        | 17     | 4     |
| 1:A:17:LYS:NZ   | 1:A:17:LYS:CB   | 0.48     | 2.76        | 19     | 3     |
| 1:A:42:GLU:CD   | 1:A:43:PHE:N    | 0.48     | 2.71        | 12     | 4     |
| 1:A:20:TYR:CD2  | 1:A:20:TYR:C    | 0.48     | 2.91        | 11     | 4     |
| 1:A:30:SER:O    | 1:A:31:CYS:SG   | 0.48     | 2.70        | 17     | 4     |
| 1:A:32:ASP:C    | 1:A:34:GLU:N    | 0.47     | 2.72        | 12     | 9     |
| 1:A:30:SER:C    | 1:A:31:CYS:SG   | 0.47     | 2.97        | 2      | 2     |
| 1:A:20:TYR:CD1  | 1:A:20:TYR:C    | 0.47     | 2.92        | 14     | 3     |
| 1:A:14:ASP:N    | 1:A:14:ASP:OD2  | 0.47     | 2.47        | 15     | 1     |
| 1:A:41:GLU:OE1  | 1:A:41:GLU:CA   | 0.47     | 2.63        | 6      | 1     |
| 1:A:31:CYS:O    | 1:A:32:ASP:CG   | 0.46     | 2.58        | 14     | 8     |
| 1:A:28:ASN:ND2  | 1:A:28:ASN:N    | 0.46     | 2.62        | 7      | 1     |
| 1:A:40:ARG:O    | 1:A:44:HIS:ND1  | 0.46     | 2.49        | 13     | 1     |
| 1:A:31:CYS:O    | 1:A:31:CYS:SG   | 0.46     | 2.73        | 9      | 2     |
| 1:A:43:PHE:C    | 1:A:43:PHE:CD1  | 0.46     | 2.93        | 2      | 2     |
| 1:A:23:LEU:CD2  | 1:A:42:GLU:OE1  | 0.45     | 2.65        | 20     | 1     |
| 1:A:28:ASN:N    | 1:A:28:ASN:HD22 | 0.45     | 2.10        | 7      | 1     |
| 1:A:42:GLU:CD   | 1:A:42:GLU:C    | 0.44     | 2.85        | 5      | 4     |
| 1:A:21:ALA:O    | 1:A:25:ASP:CG   | 0.44     | 2.61        | 9      | 7     |
| 1:A:25:ASP:O    | 1:A:29:THR:OG1  | 0.44     | 2.36        | 19     | 4     |
| 1:A:22:GLU:N    | 1:A:22:GLU:CD   | 0.43     | 2.76        | 19     | 1     |
| 1:A:37:ALA:O    | 1:A:41:GLU:CD   | 0.43     | 2.61        | 10     | 2     |
| 1:A:26:THR:O    | 1:A:30:SER:N    | 0.43     | 2.51        | 5      | 1     |
| 1:A:39:CYS:O    | 1:A:42:GLU:OE1  | 0.43     | 2.36        | 6      | 1     |
| 1:A:32:ASP:O    | 1:A:34:GLU:N    | 0.43     | 2.51        | 12     | 2     |
| 1:A:24:ARG:O    | 1:A:28:ASN:CG   | 0.43     | 2.62        | 7      | 2     |
| 1:A:32:ASP:O    | 1:A:33:ILE:C    | 0.43     | 2.62        | 19     | 8     |
| 1:A:32:ASP:OD1  | 1:A:34:GLU:OE2  | 0.42     | 2.37        | 18     | 1     |
| 1:A:36:LEU:O    | 1:A:39:CYS:SG   | 0.42     | 2.69        | 8      | 2     |
| 1:A:37:ALA:O    | 1:A:41:GLU:OE2  | 0.42     | 2.37        | 10     | 1     |
| 1:A:25:ASP:OD1  | 1:A:25:ASP:C    | 0.42     | 2.61        | 16     | 1     |
| 1:A:35:LEU:O    | 1:A:39:CYS:N    | 0.42     | 2.50        | 4      | 1     |
| 1:A:43:PHE:C    | 1:A:43:PHE:CD2  | 0.42     | 2.98        | 9      | 1     |
| 1:A:34:GLU:N    | 1:A:34:GLU:OE1  | 0.42     | 2.53        | 10     | 1     |
| 1:A:14:ASP:OD1  | 1:A:14:ASP:C    | 0.42     | 2.62        | 7      | 1     |
| 1:A:21:ALA:O    | 1:A:25:ASP:CB   | 0.41     | 2.68        | 13     | 1     |
| 1:A:21:ALA:O    | 1:A:25:ASP:OD2  | 0.41     | 2.37        | 12     | 2     |
| 1:A:14:ASP:C    | 1:A:14:ASP:OD1  | 0.41     | 2.63        | 8      | 1     |
| 1:A:15:LEU:HD13 | 1:A:42:GLU:OE1  | 0.41     | 2.16        | 2      | 1     |
| 1:A:31:CYS:O    | 1:A:32:ASP:OD1  | 0.41     | 2.39        | 14     | 1     |

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| Atom-1       | Atom-2         | Clash(Å) | Distance(Å) | Models |       |
|--------------|----------------|----------|-------------|--------|-------|
|              |                |          |             | Worst  | Total |
| 1:A:21:ALA:O | 1:A:25:ASP:OD1 | 0.41     | 2.38        | 10     | 1     |
| 1:A:25:ASP:C | 1:A:29:THR:HG1 | 0.40     | 2.24        | 6      | 1     |
| 1:A:31:CYS:O | 1:A:32:ASP:OD2 | 0.40     | 2.39        | 17     | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed       | Favoured     | Allowed     | Outliers   | Percentiles |     |
|-----|-------|----------------|--------------|-------------|------------|-------------|-----|
| 1   | A     | 33/51 (65%)    | 28±0 (85±1%) | 5±0 (15±1%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 660/1020 (65%) | 563 (85%)    | 97 (15%)    | 0 (0%)     | 100         | 100 |

There are no Ramachandran outliers.

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

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

| Mol | Chain | Analysed      | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|---------------|--------------|------------|-------------|----|
| 1   | A     | 30/45 (67%)   | 29±1 (96±3%) | 1±1 (4±3%) | 26          | 77 |
| All | All   | 600/900 (67%) | 573 (96%)    | 27 (4%)    | 26          | 77 |

All 8 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     | 28  | ASN  | 14             |
| 1   | A     | 17  | LYS  | 4              |
| 1   | A     | 35  | LEU  | 3              |
| 1   | A     | 41  | GLU  | 2              |
| 1   | A     | 24  | ARG  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 44  | HIS  | 1              |
| 1   | A     | 14  | ASP  | 1              |
| 1   | A     | 22  | GLU  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 92% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

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

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 651 |
| Number of shifts mapped to atoms        | 651 |
| 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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 51       | $-0.24 \pm 0.37$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 48       | $0.28 \pm 0.14$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 48       | $2.35 \pm 0.16$                 | Should be applied          |
| $^{15}\text{N}$        | 48       | $-0.68 \pm 0.44$                | None needed (imprecise)    |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 430 atoms were assigned a chemical shift out of a possible 474. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 165/165 (100%) | 66/66 (100%)  | 66/66 (100%)    | 33/33 (100%)    |
| Sidechain | 233/271 (86%)  | 157/173 (91%) | 71/83 (86%)     | 5/15 (33%)      |

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|          | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 32/38 (84%)   | 16/19 (84%)    | 15/17 (88%)     | 1/2 (50%)       |
| Overall  | 430/474 (91%) | 239/258 (93%)  | 152/166 (92%)   | 39/50 (78%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 651 atoms were assigned a chemical shift out of a possible 709. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 249/254 (98%) | 102/103 (99%)  | 99/102 (97%)    | 48/49 (98%)     |
| Sidechain | 350/392 (89%) | 236/252 (94%)  | 108/121 (89%)   | 6/19 (32%)      |
| Aromatic  | 52/63 (83%)   | 26/31 (84%)    | 25/29 (86%)     | 1/3 (33%)       |
| Overall   | 651/709 (92%) | 364/386 (94%)  | 232/252 (92%)   | 55/71 (77%)     |

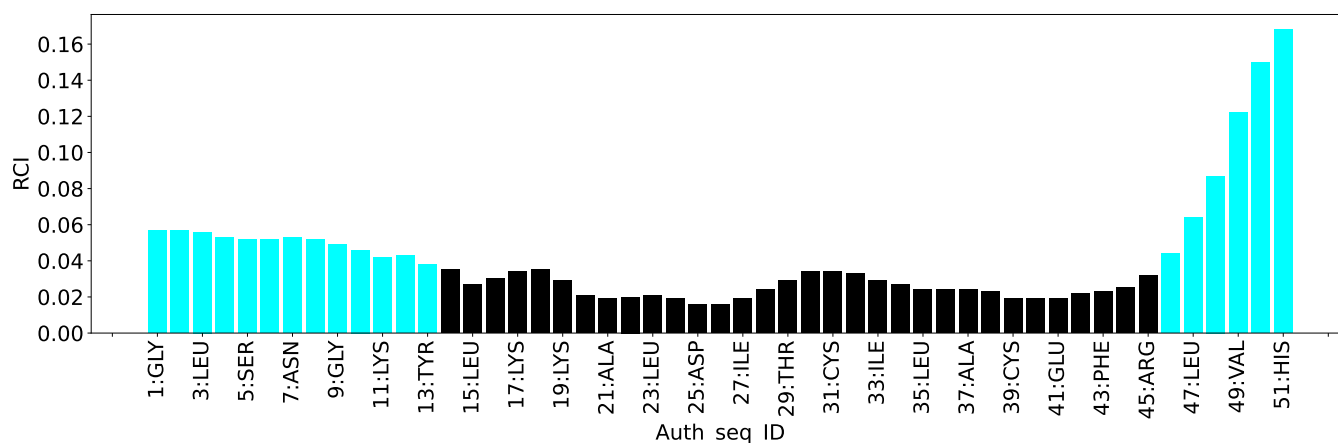
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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:



## 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                                | 890   |
| Intra-residue ( $ i-j =0$ )                              | 252   |
| Sequential ( $ i-j =1$ )                                 | 231   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 215   |
| Long range ( $ i-j \geq 5$ )                             | 110   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 82    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 54    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 18.5  |
| Number of long range restraints per residue <sup>1</sup> | 2.2   |

<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)  | 23.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 37.7                                   | 0.5     |
| >0.5 (Large)     | 9.5                                    | 3.59    |

### 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 ⓘ

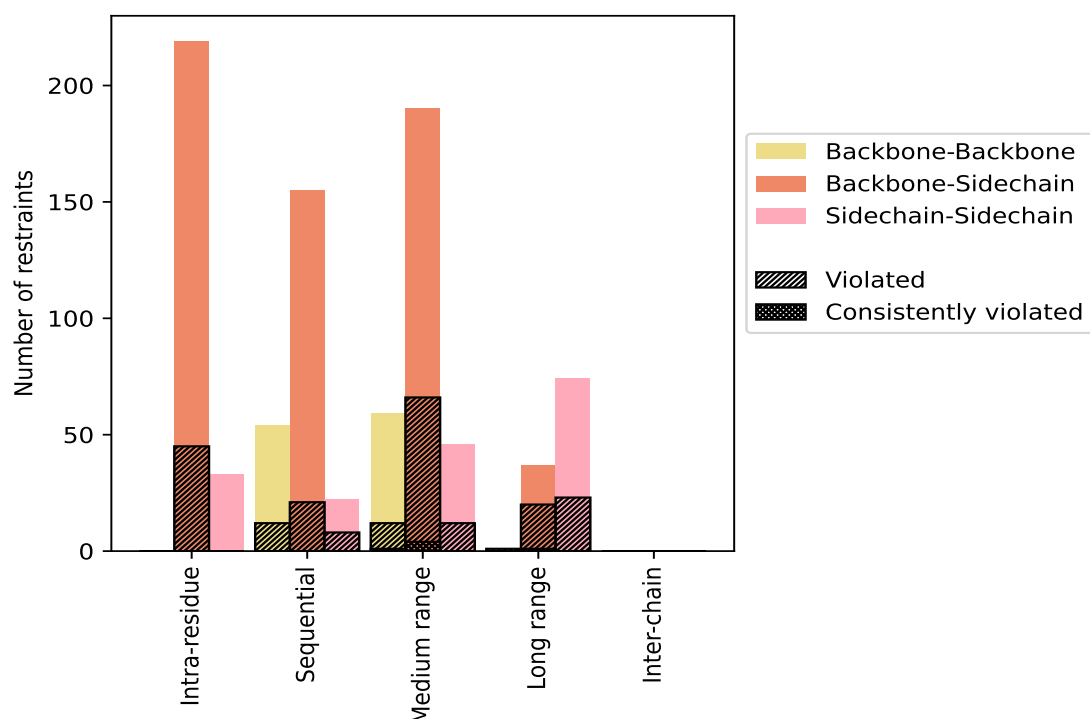
### 9.1 Summary of distance violations ⓘ

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="#">252</a> | <a href="#">28.3</a>  | <a href="#">45</a>    | <a href="#">17.9</a> | <a href="#">5.1</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                                         | 219                 | 24.6                  | 45                    | 20.5                 | 5.1                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 33                  | 3.7                   | 0                     | 0.0                  | 0.0                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Sequential ( i-j =1)</a>                       | <a href="#">231</a> | <a href="#">26.0</a>  | <a href="#">41</a>    | <a href="#">17.7</a> | <a href="#">4.6</a>  | <a href="#">0</a>                  | <a href="#">0.0</a> | <a href="#">0.0</a> |
| Backbone-Backbone                                          | 54                  | 6.1                   | 12                    | 22.2                 | 1.3                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 155                 | 17.4                  | 21                    | 13.5                 | 2.4                  | 0                                  | 0.0                 | 0.0                 |
| Sidechain-Sidechain                                        | 22                  | 2.5                   | 8                     | 36.4                 | 0.9                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a> | <a href="#">215</a> | <a href="#">24.2</a>  | <a href="#">59</a>    | <a href="#">27.4</a> | <a href="#">6.6</a>  | <a href="#">3</a>                  | <a href="#">1.4</a> | <a href="#">0.3</a> |
| Backbone-Backbone                                          | 59                  | 6.6                   | 12                    | 20.3                 | 1.3                  | 1                                  | 1.7                 | 0.1                 |
| Backbone-Sidechain                                         | 112                 | 12.6                  | 35                    | 31.2                 | 3.9                  | 2                                  | 1.8                 | 0.2                 |
| Sidechain-Sidechain                                        | 44                  | 4.9                   | 12                    | 27.3                 | 1.3                  | 0                                  | 0.0                 | 0.0                 |
| <a href="#">Long range ( i-j ≥5)</a>                       | <a href="#">110</a> | <a href="#">12.4</a>  | <a href="#">44</a>    | <a href="#">40.0</a> | <a href="#">4.9</a>  | <a href="#">1</a>                  | <a href="#">0.9</a> | <a href="#">0.1</a> |
| Backbone-Backbone                                          | 1                   | 0.1                   | 1                     | 100.0                | 0.1                  | 0                                  | 0.0                 | 0.0                 |
| Backbone-Sidechain                                         | 37                  | 4.2                   | 20                    | 54.1                 | 2.2                  | 1                                  | 2.7                 | 0.1                 |
| Sidechain-Sidechain                                        | 72                  | 8.1                   | 23                    | 31.9                 | 2.6                  | 0                                  | 0.0                 | 0.0                 |
| <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="#">82</a>  | <a href="#">9.2</a>   | <a href="#">31</a>    | <a href="#">37.8</a> | <a href="#">3.5</a>  | <a href="#">2</a>                  | <a href="#">2.4</a> | <a href="#">0.2</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="#">890</a> | <a href="#">100.0</a> | <a href="#">220</a>   | <a href="#">24.7</a> | <a href="#">24.7</a> | <a href="#">6</a>                  | <a href="#">0.7</a> | <a href="#">0.7</a> |
| Backbone-Backbone                                          | 114                 | 12.8                  | 25                    | 21.9                 | 2.8                  | 1                                  | 0.9                 | 0.1                 |
| Backbone-Sidechain                                         | 601                 | 67.5                  | 152                   | 25.3                 | 17.1                 | 5                                  | 0.8                 | 0.6                 |
| Sidechain-Sidechain                                        | 175                 | 19.7                  | 43                    | 24.6                 | 4.8                  | 0                                  | 0.0                 | 0.0                 |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 2                    | 7               | 26              | 18              | 0               | 53    | 0.34     | 2.14    | 0.37                | 0.24       |
| 2        | 9                    | 12              | 30              | 14              | 0               | 65    | 0.33     | 1.54    | 0.27                | 0.26       |
| 3        | 7                    | 10              | 45              | 15              | 0               | 77    | 0.35     | 3.02    | 0.45                | 0.24       |
| 4        | 7                    | 9               | 42              | 24              | 0               | 82    | 0.34     | 1.81    | 0.31                | 0.25       |
| 5        | 7                    | 7               | 35              | 16              | 0               | 65    | 0.36     | 3.28    | 0.51                | 0.23       |
| 6        | 4                    | 8               | 34              | 17              | 0               | 63    | 0.31     | 1.18    | 0.2                 | 0.27       |
| 7        | 9                    | 10              | 39              | 21              | 0               | 79    | 0.33     | 1.06    | 0.19                | 0.29       |
| 8        | 5                    | 7               | 41              | 19              | 0               | 72    | 0.33     | 2.4     | 0.29                | 0.27       |
| 9        | 5                    | 8               | 30              | 19              | 0               | 62    | 0.39     | 2.55    | 0.46                | 0.23       |
| 10       | 7                    | 12              | 34              | 19              | 0               | 72    | 0.32     | 1.27    | 0.24                | 0.25       |

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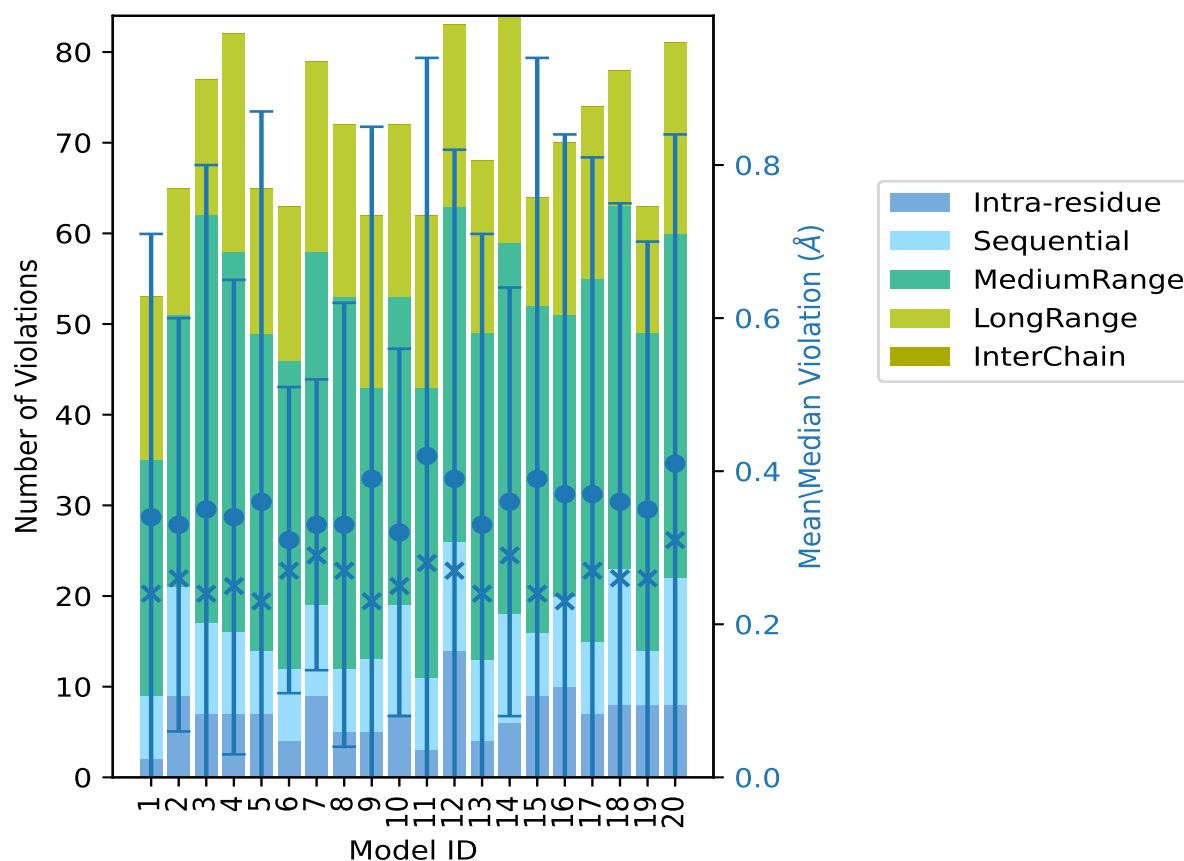
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 3                    | 8               | 32              | 19              | 0               | 62    | 0.42     | 3.36    | 0.52                | 0.28       |
| 12       | 14                   | 12              | 37              | 20              | 0               | 83    | 0.39     | 3.13    | 0.43                | 0.27       |
| 13       | 4                    | 9               | 36              | 19              | 0               | 68    | 0.33     | 2.72    | 0.38                | 0.24       |
| 14       | 6                    | 12              | 41              | 25              | 0               | 84    | 0.36     | 1.54    | 0.28                | 0.29       |
| 15       | 9                    | 7               | 36              | 12              | 0               | 64    | 0.39     | 3.59    | 0.55                | 0.24       |
| 16       | 10                   | 10              | 31              | 19              | 0               | 70    | 0.37     | 3.22    | 0.47                | 0.23       |
| 17       | 7                    | 8               | 40              | 19              | 0               | 74    | 0.37     | 3.13    | 0.44                | 0.27       |
| 18       | 8                    | 15              | 40              | 15              | 0               | 78    | 0.36     | 2.96    | 0.39                | 0.26       |
| 19       | 8                    | 6               | 35              | 14              | 0               | 63    | 0.35     | 2.29    | 0.35                | 0.26       |
| 20       | 8                    | 14              | 38              | 21              | 0               | 81    | 0.41     | 3.22    | 0.43                | 0.31       |

<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

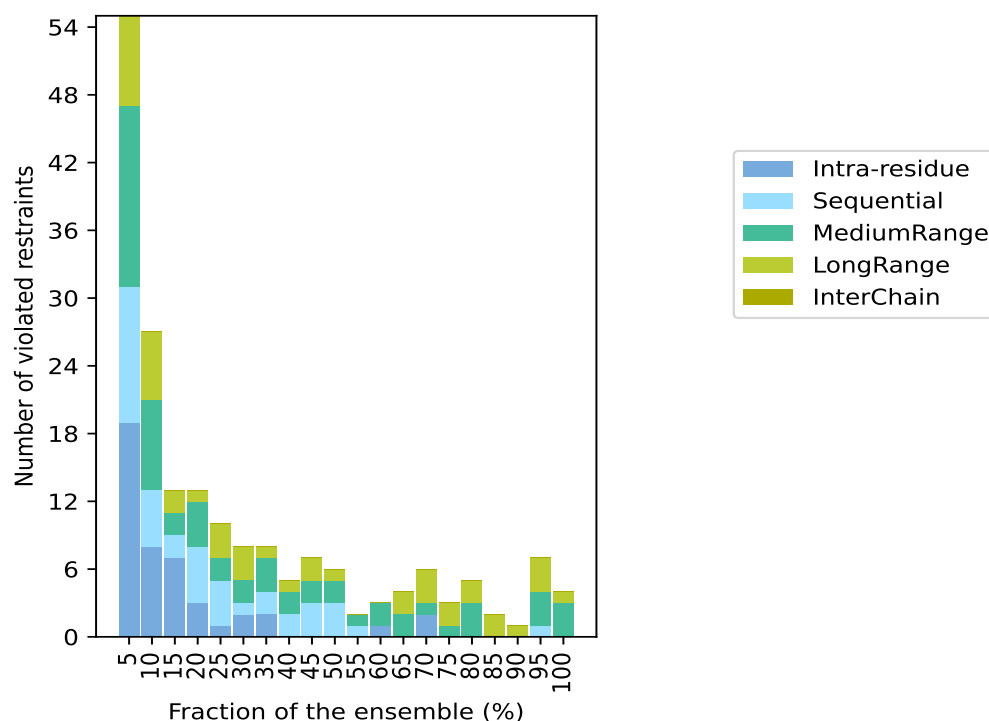
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 619(IR:207, SQ:190, MR:156, LR:66, IC:0) restraints are not 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>       | %     |
| 19                            | 12              | 16              | 8               | 0               | 55    | 1                        | 5.0   |
| 8                             | 5               | 8               | 6               | 0               | 27    | 2                        | 10.0  |
| 7                             | 2               | 2               | 2               | 0               | 13    | 3                        | 15.0  |
| 3                             | 5               | 4               | 1               | 0               | 13    | 4                        | 20.0  |
| 1                             | 4               | 2               | 3               | 0               | 10    | 5                        | 25.0  |
| 2                             | 1               | 2               | 3               | 0               | 8     | 6                        | 30.0  |
| 2                             | 2               | 3               | 1               | 0               | 8     | 7                        | 35.0  |
| 0                             | 2               | 2               | 1               | 0               | 5     | 8                        | 40.0  |
| 0                             | 3               | 2               | 2               | 0               | 7     | 9                        | 45.0  |
| 0                             | 3               | 2               | 1               | 0               | 6     | 10                       | 50.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 11                       | 55.0  |
| 1                             | 0               | 2               | 0               | 0               | 3     | 12                       | 60.0  |
| 0                             | 0               | 2               | 2               | 0               | 4     | 13                       | 65.0  |
| 2                             | 0               | 1               | 3               | 0               | 6     | 14                       | 70.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 15                       | 75.0  |
| 0                             | 0               | 3               | 2               | 0               | 5     | 16                       | 80.0  |
| 0                             | 0               | 0               | 2               | 0               | 2     | 17                       | 85.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 18                       | 90.0  |
| 0                             | 1               | 3               | 3               | 0               | 7     | 19                       | 95.0  |
| 0                             | 0               | 3               | 1               | 0               | 4     | 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

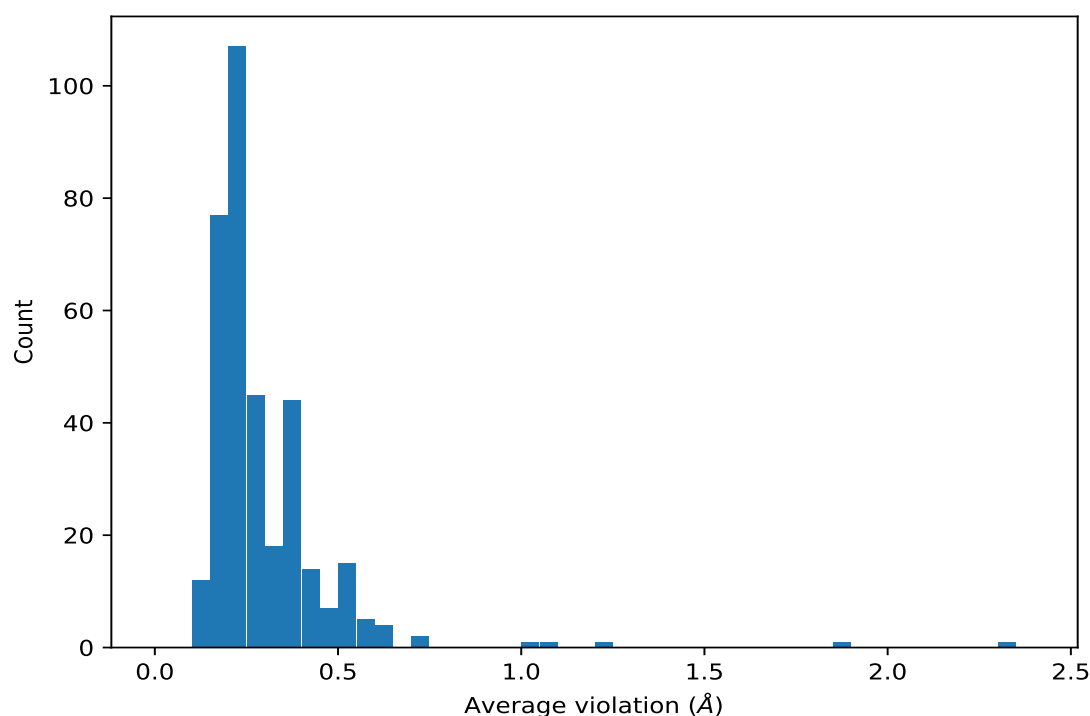
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,39)  | 1:49:A:VAL:H    | 1:45:A:ARG:O    | 20                  | 2.31     | 0.99                | 2.64       |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 20                  | 0.54     | 0.12                | 0.55       |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 20                  | 0.54     | 0.12                | 0.55       |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 20                  | 0.54     | 0.12                | 0.55       |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 20                  | 0.49     | 0.04                | 0.5        |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 20                  | 0.44     | 0.09                | 0.48       |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 20                  | 0.32     | 0.11                | 0.34       |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 20                  | 0.32     | 0.11                | 0.34       |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 20                  | 0.32     | 0.11                | 0.34       |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 20                  | 0.3      | 0.0                 | 0.3        |
| (1,115) | 1:47:A:LEU:H    | 1:49:A:VAL:H    | 19                  | 1.87     | 0.61                | 2.0        |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD11 | 19                  | 0.6      | 0.06                | 0.63       |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD12 | 19                  | 0.6      | 0.06                | 0.63       |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD13 | 19                  | 0.6      | 0.06                | 0.63       |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 19                  | 0.43     | 0.1                 | 0.5        |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 19                  | 0.43     | 0.1                 | 0.5        |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 19                  | 0.43     | 0.1                 | 0.5        |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 19                  | 0.35     | 0.12                | 0.35       |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 19                  | 0.35     | 0.1                 | 0.38       |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 19                  | 0.28     | 0.14                | 0.27       |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 19                  | 0.28     | 0.14                | 0.27       |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 19                  | 0.28     | 0.14                | 0.27       |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 19                  | 0.26     | 0.08                | 0.29       |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 18                  | 0.31     | 0.13                | 0.29       |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 18                  | 0.31     | 0.13                | 0.29       |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 18                  | 0.31     | 0.13                | 0.29       |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 18                  | 0.14     | 0.02                | 0.15       |
| (2,40)  | 1:49:A:VAL:N    | 1:45:A:ARG:O    | 17                  | 1.07     | 0.46                | 1.24       |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 17                  | 0.37     | 0.13                | 0.37       |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 17                  | 0.37     | 0.13                | 0.37       |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 17                  | 0.37     | 0.13                | 0.37       |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 17                  | 0.26     | 0.06                | 0.28       |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 17                  | 0.25     | 0.05                | 0.26       |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 17                  | 0.2      | 0.02                | 0.21       |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 17                  | 0.2      | 0.02                | 0.21       |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 17                  | 0.2      | 0.02                | 0.21       |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 17                  | 0.2      | 0.02                | 0.21       |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 17                  | 0.2      | 0.02                | 0.21       |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 17                  | 0.2      | 0.02                | 0.21       |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 17                  | 0.2      | 0.02                | 0.21       |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 17                  | 0.2      | 0.02                | 0.21       |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 17                  | 0.2      | 0.02                | 0.21       |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 17                  | 0.19     | 0.05                | 0.2        |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 16                  | 0.61     | 0.19                | 0.68       |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 16                  | 0.45     | 0.08                | 0.5        |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 16                  | 0.45     | 0.08                | 0.5        |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 16                  | 0.29     | 0.03                | 0.3        |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 16                  | 0.29     | 0.03                | 0.3        |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 16                  | 0.29     | 0.03                | 0.3        |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 16                  | 0.26     | 0.06                | 0.28       |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 16                  | 0.26     | 0.07                | 0.25       |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 16                  | 0.24     | 0.08                | 0.22       |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 16                  | 0.24     | 0.08                | 0.22       |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 16                  | 0.23     | 0.04                | 0.25       |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 16                  | 0.23     | 0.06                | 0.26       |
| (1,23)  | 1:30:A:SER:HG   | 1:32:A:ASP:H    | 15                  | 1.21     | 0.53                | 1.32       |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 15                  | 0.39     | 0.12                | 0.46       |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 15                  | 0.39     | 0.12                | 0.46       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 15                  | 0.39     | 0.12                | 0.46       |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 15                  | 0.39     | 0.12                | 0.46       |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 15                  | 0.39     | 0.12                | 0.46       |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 15                  | 0.39     | 0.12                | 0.46       |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 15                  | 0.24     | 0.07                | 0.23       |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 15                  | 0.24     | 0.07                | 0.23       |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 15                  | 0.24     | 0.07                | 0.23       |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 15                  | 0.24     | 0.06                | 0.28       |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 15                  | 0.22     | 0.05                | 0.24       |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD2  | 14                  | 0.73     | 0.3                 | 0.75       |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD3  | 14                  | 0.73     | 0.3                 | 0.75       |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 14                  | 0.52     | 0.05                | 0.54       |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 14                  | 0.52     | 0.05                | 0.54       |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 14                  | 0.35     | 0.15                | 0.37       |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 14                  | 0.35     | 0.15                | 0.37       |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 14                  | 0.35     | 0.15                | 0.37       |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 14                  | 0.28     | 0.09                | 0.24       |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 14                  | 0.28     | 0.09                | 0.24       |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 14                  | 0.28     | 0.09                | 0.24       |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 14                  | 0.28     | 0.09                | 0.24       |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 14                  | 0.28     | 0.09                | 0.24       |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 14                  | 0.28     | 0.09                | 0.24       |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 14                  | 0.23     | 0.06                | 0.22       |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 14                  | 0.23     | 0.06                | 0.22       |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 14                  | 0.23     | 0.06                | 0.22       |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 14                  | 0.22     | 0.02                | 0.23       |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 13                  | 0.27     | 0.13                | 0.23       |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 13                  | 0.27     | 0.13                | 0.23       |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 13                  | 0.27     | 0.13                | 0.23       |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 13                  | 0.23     | 0.13                | 0.14       |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 13                  | 0.23     | 0.13                | 0.14       |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 13                  | 0.23     | 0.13                | 0.14       |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD11 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD12 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD13 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD21 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD22 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD23 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD11 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD12 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD13 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD21 | 13                  | 0.2      | 0.02                | 0.21       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD22 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD23 | 13                  | 0.2      | 0.02                | 0.21       |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 13                  | 0.19     | 0.07                | 0.22       |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 13                  | 0.19     | 0.07                | 0.22       |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 13                  | 0.19     | 0.07                | 0.22       |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 13                  | 0.19     | 0.04                | 0.18       |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 12                  | 0.36     | 0.11                | 0.36       |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 12                  | 0.27     | 0.01                | 0.27       |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 12                  | 0.23     | 0.08                | 0.22       |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 12                  | 0.16     | 0.04                | 0.16       |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 11                  | 0.28     | 0.16                | 0.24       |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 11                  | 0.26     | 0.14                | 0.21       |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 11                  | 0.26     | 0.14                | 0.21       |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD21 | 10                  | 0.56     | 0.33                | 0.44       |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD22 | 10                  | 0.56     | 0.33                | 0.44       |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD23 | 10                  | 0.56     | 0.33                | 0.44       |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 10                  | 0.44     | 0.2                 | 0.5        |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 10                  | 0.44     | 0.2                 | 0.5        |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 10                  | 0.44     | 0.2                 | 0.5        |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 10                  | 0.29     | 0.12                | 0.26       |
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 10                  | 0.2      | 0.07                | 0.2        |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 10                  | 0.18     | 0.03                | 0.2        |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD11 | 10                  | 0.18     | 0.05                | 0.18       |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD12 | 10                  | 0.18     | 0.05                | 0.18       |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD13 | 10                  | 0.18     | 0.05                | 0.18       |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD21 | 10                  | 0.18     | 0.05                | 0.18       |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD22 | 10                  | 0.18     | 0.05                | 0.18       |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD23 | 10                  | 0.18     | 0.05                | 0.18       |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 10                  | 0.15     | 0.04                | 0.14       |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 10                  | 0.15     | 0.04                | 0.14       |
| (1,185) | 1:26:A:THR:HG1  | 1:27:A:ILE:H    | 9                   | 0.34     | 0.06                | 0.33       |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 9                   | 0.31     | 0.12                | 0.34       |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 9                   | 0.27     | 0.07                | 0.29       |
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 9                   | 0.26     | 0.12                | 0.33       |
| (2,37)  | 1:48:A:LYS:H    | 1:44:A:HIS:O    | 9                   | 0.22     | 0.07                | 0.23       |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 9                   | 0.21     | 0.03                | 0.2        |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 9                   | 0.2      | 0.07                | 0.18       |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 9                   | 0.18     | 0.05                | 0.15       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 9                   | 0.18     | 0.05                | 0.15       |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 9                   | 0.16     | 0.03                | 0.16       |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 9                   | 0.16     | 0.03                | 0.16       |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 9                   | 0.16     | 0.03                | 0.16       |
| (1,279) | 1:44:A:HIS:HD2  | 1:45:A:ARG:H    | 8                   | 0.52     | 0.25                | 0.6        |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 8                   | 0.41     | 0.11                | 0.46       |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 8                   | 0.41     | 0.11                | 0.46       |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 8                   | 0.41     | 0.11                | 0.46       |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 8                   | 0.41     | 0.11                | 0.46       |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 8                   | 0.41     | 0.11                | 0.46       |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 8                   | 0.41     | 0.11                | 0.46       |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 8                   | 0.31     | 0.12                | 0.3        |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 8                   | 0.27     | 0.07                | 0.26       |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 8                   | 0.27     | 0.07                | 0.26       |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB1  | 8                   | 0.18     | 0.05                | 0.16       |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB2  | 8                   | 0.18     | 0.05                | 0.16       |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB3  | 8                   | 0.18     | 0.05                | 0.16       |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 8                   | 0.15     | 0.04                | 0.14       |
| (1,182) | 1:25:A:ASP:HA   | 1:28:A:ASN:HD21 | 7                   | 0.35     | 0.13                | 0.37       |
| (1,664) | 1:12:A:LYS:HB2  | 1:13:A:TYR:H    | 7                   | 0.31     | 0.07                | 0.33       |
| (1,664) | 1:12:A:LYS:HB3  | 1:13:A:TYR:H    | 7                   | 0.31     | 0.07                | 0.33       |
| (1,534) | 1:44:A:HIS:HA   | 1:44:A:HIS:HD2  | 7                   | 0.27     | 0.09                | 0.26       |
| (1,110) | 1:49:A:VAL:H    | 1:49:A:VAL:HB   | 7                   | 0.25     | 0.06                | 0.26       |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD11 | 7                   | 0.18     | 0.08                | 0.16       |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD12 | 7                   | 0.18     | 0.08                | 0.16       |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD13 | 7                   | 0.18     | 0.08                | 0.16       |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD11 | 7                   | 0.18     | 0.08                | 0.16       |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD12 | 7                   | 0.18     | 0.08                | 0.16       |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD13 | 7                   | 0.18     | 0.08                | 0.16       |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD11 | 7                   | 0.18     | 0.08                | 0.16       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD12 | 7                   | 0.18     | 0.08                | 0.16       |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD13 | 7                   | 0.18     | 0.08                | 0.16       |
| (1,268) | 1:38:A:ALA:H    | 1:41:A:GLU:H    | 7                   | 0.15     | 0.03                | 0.14       |
| (1,88)  | 1:41:A:GLU:HA   | 1:45:A:ARG:H    | 7                   | 0.14     | 0.03                | 0.16       |
| (1,148) | 1:15:A:LEU:H    | 1:16:A:SER:H    | 7                   | 0.13     | 0.01                | 0.13       |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG21 | 6                   | 0.51     | 0.01                | 0.51       |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG22 | 6                   | 0.51     | 0.01                | 0.51       |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG23 | 6                   | 0.51     | 0.01                | 0.51       |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG21 | 6                   | 0.51     | 0.01                | 0.51       |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG22 | 6                   | 0.51     | 0.01                | 0.51       |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG23 | 6                   | 0.51     | 0.01                | 0.51       |
| (1,414) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HA   | 6                   | 0.36     | 0.13                | 0.38       |
| (1,414) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HA   | 6                   | 0.36     | 0.13                | 0.38       |
| (1,595) | 1:24:A:ARG:HA   | 1:24:A:ARG:HD3  | 6                   | 0.34     | 0.04                | 0.34       |
| (1,170) | 1:28:A:ASN:HB2  | 1:30:A:SER:H    | 6                   | 0.27     | 0.14                | 0.27       |
| (2,4)   | 1:24:A:ARG:N    | 1:20:A:TYR:O    | 6                   | 0.21     | 0.05                | 0.22       |
| (1,36)  | 1:11:A:LYS:H    | 1:12:A:LYS:H    | 6                   | 0.2      | 0.03                | 0.2        |
| (1,273) | 1:27:A:ILE:HD11 | 1:43:A:PHE:H    | 6                   | 0.2      | 0.04                | 0.2        |
| (1,273) | 1:27:A:ILE:HD12 | 1:43:A:PHE:H    | 6                   | 0.2      | 0.04                | 0.2        |
| (1,273) | 1:27:A:ILE:HD13 | 1:43:A:PHE:H    | 6                   | 0.2      | 0.04                | 0.2        |
| (1,491) | 1:27:A:ILE:HA   | 1:32:A:ASP:H    | 6                   | 0.2      | 0.02                | 0.2        |
| (2,12)  | 1:28:A:ASN:N    | 1:24:A:ARG:O    | 6                   | 0.16     | 0.05                | 0.14       |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB2  | 6                   | 0.15     | 0.02                | 0.15       |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 6                   | 0.15     | 0.02                | 0.15       |
| (2,10)  | 1:27:A:ILE:N    | 1:23:A:LEU:O    | 6                   | 0.14     | 0.02                | 0.14       |
| (2,26)  | 1:41:A:GLU:N    | 1:37:A:ALA:O    | 6                   | 0.12     | 0.01                | 0.12       |
| (1,165) | 1:3:A:LEU:H     | 1:4:A:GLY:H     | 5                   | 0.41     | 0.09                | 0.4        |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE1  | 5                   | 0.39     | 0.15                | 0.49       |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE2  | 5                   | 0.39     | 0.15                | 0.49       |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE1  | 5                   | 0.39     | 0.15                | 0.49       |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE2  | 5                   | 0.39     | 0.15                | 0.49       |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG11 | 5                   | 0.36     | 0.07                | 0.34       |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG12 | 5                   | 0.36     | 0.07                | 0.34       |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG13 | 5                   | 0.36     | 0.07                | 0.34       |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG21 | 5                   | 0.36     | 0.07                | 0.34       |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG22 | 5                   | 0.36     | 0.07                | 0.34       |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG23 | 5                   | 0.36     | 0.07                | 0.34       |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD2  | 5                   | 0.35     | 0.12                | 0.32       |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD3  | 5                   | 0.35     | 0.12                | 0.32       |
| (1,361) | 1:49:A:VAL:HA   | 1:50:A:TYR:H    | 5                   | 0.22     | 0.06                | 0.22       |
| (1,634) | 1:29:A:THR:H    | 1:30:A:SER:HB3  | 5                   | 0.22     | 0.17                | 0.13       |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD21 | 5                   | 0.18     | 0.05                | 0.17       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD22 | 5                   | 0.18     | 0.05                | 0.17       |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD23 | 5                   | 0.18     | 0.05                | 0.17       |
| (1,392) | 1:18:A:TRP:HZ3  | 1:23:A:LEU:HA   | 5                   | 0.18     | 0.07                | 0.16       |
| (1,91)  | 1:34:A:GLU:HA   | 1:37:A:ALA:H    | 5                   | 0.15     | 0.05                | 0.12       |
| (1,41)  | 1:2:A:PRO:HA    | 1:3:A:LEU:H     | 5                   | 0.13     | 0.01                | 0.13       |
| (1,37)  | 1:11:A:LYS:HA   | 1:12:A:LYS:H    | 4                   | 0.36     | 0.09                | 0.33       |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE1  | 4                   | 0.28     | 0.07                | 0.26       |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE2  | 4                   | 0.28     | 0.07                | 0.26       |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE1  | 4                   | 0.28     | 0.07                | 0.26       |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE2  | 4                   | 0.28     | 0.07                | 0.26       |
| (1,13)  | 1:50:A:TYR:HA   | 1:51:A:HIS:H    | 4                   | 0.28     | 0.05                | 0.3        |
| (2,13)  | 1:29:A:THR:H    | 1:25:A:ASP:O    | 4                   | 0.28     | 0.04                | 0.3        |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB2  | 4                   | 0.27     | 0.08                | 0.29       |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB3  | 4                   | 0.27     | 0.08                | 0.29       |
| (2,5)   | 1:25:A:ASP:H    | 1:21:A:ALA:O    | 4                   | 0.26     | 0.04                | 0.26       |
| (1,431) | 1:21:A:ALA:HA   | 1:24:A:ARG:HB2  | 4                   | 0.24     | 0.04                | 0.24       |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG11 | 4                   | 0.24     | 0.1                 | 0.24       |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG12 | 4                   | 0.24     | 0.1                 | 0.24       |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG13 | 4                   | 0.24     | 0.1                 | 0.24       |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG21 | 4                   | 0.24     | 0.1                 | 0.24       |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG22 | 4                   | 0.24     | 0.1                 | 0.24       |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG23 | 4                   | 0.24     | 0.1                 | 0.24       |
| (1,199) | 1:19:A:LYS:HA   | 1:21:A:ALA:H    | 4                   | 0.21     | 0.05                | 0.24       |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB1  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB2  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB3  | 4                   | 0.21     | 0.07                | 0.22       |
| (1,42)  | 1:3:A:LEU:H     | 1:3:A:LEU:HG    | 4                   | 0.2      | 0.06                | 0.22       |
| (1,644) | 1:48:A:LYS:HD2  | 1:49:A:VAL:H    | 4                   | 0.2      | 0.06                | 0.22       |
| (1,644) | 1:48:A:LYS:HD3  | 1:49:A:VAL:H    | 4                   | 0.2      | 0.06                | 0.22       |
| (2,38)  | 1:48:A:LYS:N    | 1:44:A:HIS:O    | 4                   | 0.18     | 0.05                | 0.19       |
| (1,277) | 1:44:A:HIS:H    | 1:44:A:HIS:HD2  | 4                   | 0.17     | 0.03                | 0.18       |
| (1,463) | 1:15:A:LEU:HD21 | 1:18:A:TRP:HE3  | 4                   | 0.16     | 0.08                | 0.12       |
| (1,463) | 1:15:A:LEU:HD22 | 1:18:A:TRP:HE3  | 4                   | 0.16     | 0.08                | 0.12       |
| (1,463) | 1:15:A:LEU:HD23 | 1:18:A:TRP:HE3  | 4                   | 0.16     | 0.08                | 0.12       |
| (2,19)  | 1:38:A:ALA:H    | 1:34:A:GLU:O    | 4                   | 0.15     | 0.04                | 0.13       |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD21 | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD22 | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD23 | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,734) | 1:38:A:ALA:H    | 1:41:A:GLU:HG2  | 3                   | 0.55     | 0.12                | 0.56       |
| (1,734) | 1:38:A:ALA:H    | 1:41:A:GLU:HG3  | 3                   | 0.55     | 0.12                | 0.56       |
| (1,743) | 1:39:A:CYS:HB2  | 1:40:A:ARG:HB2  | 3                   | 0.48     | 0.01                | 0.48       |
| (1,743) | 1:39:A:CYS:HB2  | 1:40:A:ARG:HB3  | 3                   | 0.48     | 0.01                | 0.48       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,743) | 1:39:A:CYS:HB3  | 1:40:A:ARG:HB2  | 3                   | 0.48     | 0.01                | 0.48       |
| (1,743) | 1:39:A:CYS:HB3  | 1:40:A:ARG:HB3  | 3                   | 0.48     | 0.01                | 0.48       |
| (1,21)  | 1:35:A:LEU:H    | 1:35:A:LEU:HG   | 3                   | 0.39     | 0.09                | 0.33       |
| (1,330) | 1:20:A:TYR:HE1  | 1:24:A:ARG:HD2  | 3                   | 0.37     | 0.05                | 0.38       |
| (1,330) | 1:20:A:TYR:HE2  | 1:24:A:ARG:HD2  | 3                   | 0.37     | 0.05                | 0.38       |
| (1,162) | 1:10:A:THR:H    | 1:10:A:THR:HB   | 3                   | 0.32     | 0.01                | 0.32       |
| (1,751) | 1:41:A:GLU:H    | 1:41:A:GLU:HG2  | 3                   | 0.3      | 0.18                | 0.18       |
| (1,751) | 1:41:A:GLU:H    | 1:41:A:GLU:HG3  | 3                   | 0.3      | 0.18                | 0.18       |
| (1,26)  | 1:10:A:THR:HA   | 1:11:A:LYS:H    | 3                   | 0.28     | 0.15                | 0.26       |
| (1,661) | 1:12:A:LYS:H    | 1:12:A:LYS:HB2  | 3                   | 0.28     | 0.02                | 0.27       |
| (1,661) | 1:12:A:LYS:H    | 1:12:A:LYS:HB3  | 3                   | 0.28     | 0.02                | 0.27       |
| (2,23)  | 1:40:A:ARG:H    | 1:36:A:LEU:O    | 3                   | 0.26     | 0.04                | 0.28       |
| (1,101) | 1:41:A:GLU:H    | 1:41:A:GLU:HG3  | 3                   | 0.24     | 0.17                | 0.13       |
| (1,776) | 1:45:A:ARG:H    | 1:45:A:ARG:HG2  | 3                   | 0.23     | 0.02                | 0.25       |
| (1,776) | 1:45:A:ARG:H    | 1:45:A:ARG:HG3  | 3                   | 0.23     | 0.02                | 0.25       |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD11 | 3                   | 0.23     | 0.07                | 0.21       |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD12 | 3                   | 0.23     | 0.07                | 0.21       |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD13 | 3                   | 0.23     | 0.07                | 0.21       |
| (1,254) | 1:15:A:LEU:HD11 | 1:39:A:CYS:H    | 3                   | 0.2      | 0.07                | 0.21       |
| (1,254) | 1:15:A:LEU:HD12 | 1:39:A:CYS:H    | 3                   | 0.2      | 0.07                | 0.21       |
| (1,254) | 1:15:A:LEU:HD13 | 1:39:A:CYS:H    | 3                   | 0.2      | 0.07                | 0.21       |
| (1,509) | 1:19:A:LYS:HA   | 1:19:A:LYS:HD2  | 3                   | 0.15     | 0.05                | 0.13       |
| (2,24)  | 1:40:A:ARG:N    | 1:36:A:LEU:O    | 3                   | 0.15     | 0.03                | 0.17       |
| (1,141) | 1:29:A:THR:HB   | 1:30:A:SER:H    | 2                   | 1.02     | 0.01                | 1.02       |
| (1,145) | 1:26:A:THR:HG21 | 1:30:A:SER:H    | 2                   | 0.5      | 0.01                | 0.5        |
| (1,145) | 1:26:A:THR:HG22 | 1:30:A:SER:H    | 2                   | 0.5      | 0.01                | 0.5        |
| (1,145) | 1:26:A:THR:HG23 | 1:30:A:SER:H    | 2                   | 0.5      | 0.01                | 0.5        |
| (1,348) | 1:41:A:GLU:H    | 1:41:A:GLU:HG2  | 2                   | 0.38     | 0.26                | 0.38       |
| (1,379) | 1:45:A:ARG:H    | 1:45:A:ARG:HG3  | 2                   | 0.38     | 0.0                 | 0.38       |
| (1,805) | 1:49:A:VAL:HG11 | 1:51:A:HIS:H    | 2                   | 0.37     | 0.01                | 0.37       |
| (1,805) | 1:49:A:VAL:HG12 | 1:51:A:HIS:H    | 2                   | 0.37     | 0.01                | 0.37       |
| (1,805) | 1:49:A:VAL:HG13 | 1:51:A:HIS:H    | 2                   | 0.37     | 0.01                | 0.37       |
| (1,805) | 1:49:A:VAL:HG21 | 1:51:A:HIS:H    | 2                   | 0.37     | 0.01                | 0.37       |
| (1,805) | 1:49:A:VAL:HG22 | 1:51:A:HIS:H    | 2                   | 0.37     | 0.01                | 0.37       |
| (1,805) | 1:49:A:VAL:HG23 | 1:51:A:HIS:H    | 2                   | 0.37     | 0.01                | 0.37       |
| (1,12)  | 1:51:A:HIS:H    | 1:51:A:HIS:HD2  | 2                   | 0.36     | 0.01                | 0.36       |
| (1,89)  | 1:45:A:ARG:H    | 1:45:A:ARG:HG2  | 2                   | 0.36     | 0.02                | 0.36       |
| (1,544) | 1:32:A:ASP:HB3  | 1:35:A:LEU:HG   | 2                   | 0.32     | 0.02                | 0.32       |
| (1,143) | 1:26:A:THR:HA   | 1:30:A:SER:H    | 2                   | 0.3      | 0.02                | 0.3        |
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD21 | 2                   | 0.24     | 0.04                | 0.24       |
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD22 | 2                   | 0.24     | 0.04                | 0.24       |
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD23 | 2                   | 0.24     | 0.04                | 0.24       |

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| Key     | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD21 | 2                   | 0.24     | 0.04                | 0.24       |
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD22 | 2                   | 0.24     | 0.04                | 0.24       |
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD23 | 2                   | 0.24     | 0.04                | 0.24       |
| (1,453) | 1:10:A:THR:HG21 | 1:11:A:LYS:H    | 2                   | 0.24     | 0.01                | 0.24       |
| (1,453) | 1:10:A:THR:HG22 | 1:11:A:LYS:H    | 2                   | 0.24     | 0.01                | 0.24       |
| (1,453) | 1:10:A:THR:HG23 | 1:11:A:LYS:H    | 2                   | 0.24     | 0.01                | 0.24       |
| (1,324) | 1:27:A:ILE:HD11 | 1:43:A:PHE:HD1  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,324) | 1:27:A:ILE:HD11 | 1:43:A:PHE:HD2  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,324) | 1:27:A:ILE:HD12 | 1:43:A:PHE:HD1  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,324) | 1:27:A:ILE:HD12 | 1:43:A:PHE:HD2  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,324) | 1:27:A:ILE:HD13 | 1:43:A:PHE:HD1  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,324) | 1:27:A:ILE:HD13 | 1:43:A:PHE:HD2  | 2                   | 0.23     | 0.04                | 0.23       |
| (1,241) | 1:13:A:TYR:HE1  | 1:35:A:LEU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,241) | 1:13:A:TYR:HE2  | 1:35:A:LEU:H    | 2                   | 0.22     | 0.1                 | 0.22       |
| (1,679) | 1:17:A:LYS:H    | 1:17:A:LYS:HG2  | 2                   | 0.21     | 0.0                 | 0.21       |
| (1,679) | 1:17:A:LYS:H    | 1:17:A:LYS:HG3  | 2                   | 0.21     | 0.0                 | 0.21       |
| (1,731) | 1:37:A:ALA:HA   | 1:40:A:ARG:HD2  | 2                   | 0.21     | 0.1                 | 0.21       |
| (1,731) | 1:37:A:ALA:HA   | 1:40:A:ARG:HD3  | 2                   | 0.21     | 0.1                 | 0.21       |
| (1,183) | 1:27:A:ILE:H    | 1:28:A:ASN:HB2  | 2                   | 0.2      | 0.03                | 0.2        |
| (1,249) | 1:15:A:LEU:HD11 | 1:38:A:ALA:H    | 2                   | 0.2      | 0.07                | 0.2        |
| (1,249) | 1:15:A:LEU:HD12 | 1:38:A:ALA:H    | 2                   | 0.2      | 0.07                | 0.2        |
| (1,249) | 1:15:A:LEU:HD13 | 1:38:A:ALA:H    | 2                   | 0.2      | 0.07                | 0.2        |
| (1,624) | 1:15:A:LEU:HD11 | 1:39:A:CYS:HA   | 2                   | 0.2      | 0.01                | 0.2        |
| (1,624) | 1:15:A:LEU:HD12 | 1:39:A:CYS:HA   | 2                   | 0.2      | 0.01                | 0.2        |
| (1,624) | 1:15:A:LEU:HD13 | 1:39:A:CYS:HA   | 2                   | 0.2      | 0.01                | 0.2        |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB1  | 2                   | 0.2      | 0.01                | 0.2        |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB2  | 2                   | 0.2      | 0.01                | 0.2        |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB3  | 2                   | 0.2      | 0.01                | 0.2        |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB1  | 2                   | 0.2      | 0.01                | 0.2        |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB2  | 2                   | 0.2      | 0.01                | 0.2        |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB3  | 2                   | 0.2      | 0.01                | 0.2        |
| (1,640) | 1:19:A:LYS:HA   | 1:19:A:LYS:HD3  | 2                   | 0.17     | 0.03                | 0.17       |
| (1,754) | 1:41:A:GLU:HA   | 1:44:A:HIS:HB2  | 2                   | 0.17     | 0.01                | 0.17       |
| (1,754) | 1:41:A:GLU:HA   | 1:44:A:HIS:HB3  | 2                   | 0.17     | 0.01                | 0.17       |
| (1,226) | 1:26:A:THR:HG21 | 1:31:A:CYS:H    | 2                   | 0.16     | 0.04                | 0.16       |
| (1,226) | 1:26:A:THR:HG22 | 1:31:A:CYS:H    | 2                   | 0.16     | 0.04                | 0.16       |
| (1,226) | 1:26:A:THR:HG23 | 1:31:A:CYS:H    | 2                   | 0.16     | 0.04                | 0.16       |
| (1,685) | 1:19:A:LYS:H    | 1:19:A:LYS:HD2  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,685) | 1:19:A:LYS:H    | 1:19:A:LYS:HD3  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,168) | 1:27:A:ILE:HA   | 1:29:A:THR:H    | 2                   | 0.16     | 0.0                 | 0.16       |
| (1,301) | 1:17:A:LYS:H    | 1:18:A:TRP:HB2  | 2                   | 0.15     | 0.03                | 0.15       |
| (1,144) | 1:30:A:SER:H    | 1:30:A:SER:HB2  | 2                   | 0.15     | 0.02                | 0.15       |

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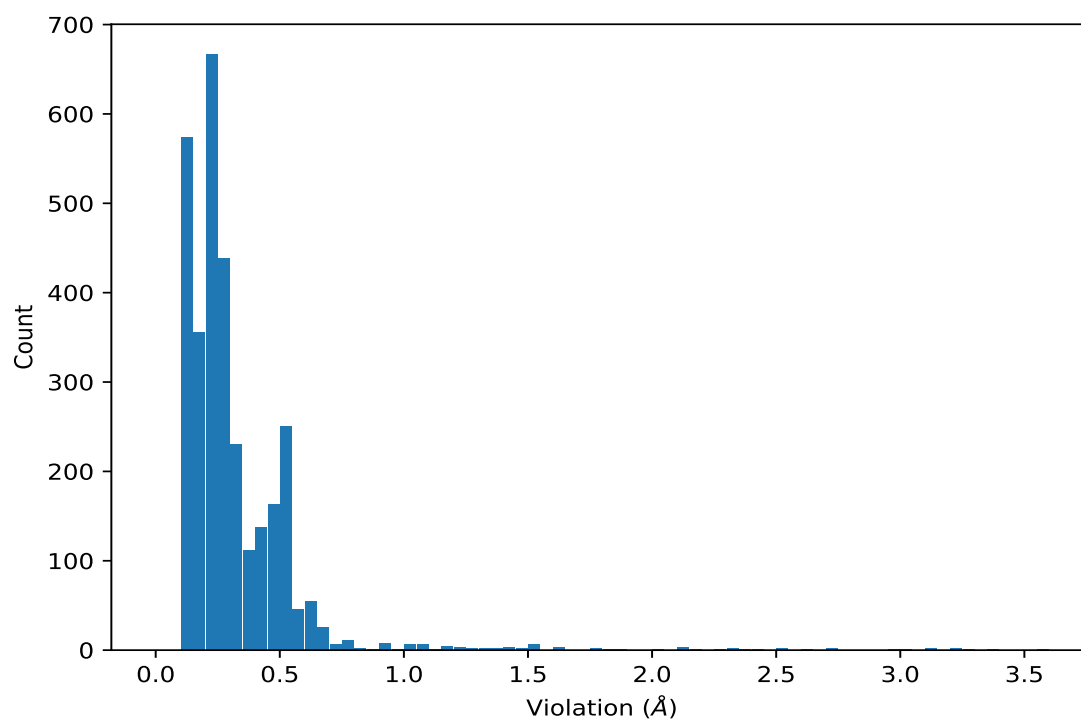
| Key     | Atom-1       | Atom-2       | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|--------------|--------------|---------------------|----------|---------------------|------------|
| (2,20)  | 1:38:A:ALA:N | 1:34:A:GLU:O | 2                   | 0.14     | 0.04                | 0.14       |
| (2,6)   | 1:25:A:ASP:N | 1:21:A:ALA:O | 2                   | 0.14     | 0.02                | 0.14       |
| (1,109) | 1:49:A:VAL:H | 1:50:A:TYR:H | 2                   | 0.12     | 0.0                 | 0.12       |

<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) |
|--------|--------------|--------------|----------|---------------|
| (2,39) | 1:49:A:VAL:H | 1:45:A:ARG:O | 15       | 3.59          |

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| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 11       | 3.36          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 5        | 3.28          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 16       | 3.22          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 20       | 3.22          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 12       | 3.13          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 17       | 3.13          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 3        | 3.02          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 18       | 2.96          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 13       | 2.72          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 3        | 2.71          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 15       | 2.64          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 9        | 2.55          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 9        | 2.53          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 5        | 2.43          |
| (1,23)  | 1:30:A:SER:HG | 1:32:A:ASP:H | 8        | 2.4           |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 12       | 2.34          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 16       | 2.33          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 19       | 2.29          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 17       | 2.17          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 1        | 2.14          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 11       | 2.13          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 20       | 2.12          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 19       | 2.0           |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 1        | 1.9           |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 4        | 1.81          |
| (2,40)  | 1:49:A:VAL:N  | 1:45:A:ARG:O | 15       | 1.78          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 4        | 1.78          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 18       | 1.63          |
| (2,40)  | 1:49:A:VAL:N  | 1:45:A:ARG:O | 11       | 1.62          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 13       | 1.62          |
| (1,115) | 1:47:A:LEU:H  | 1:49:A:VAL:H | 14       | 1.54          |
| (1,23)  | 1:30:A:SER:HG | 1:32:A:ASP:H | 2        | 1.54          |
| (1,23)  | 1:30:A:SER:HG | 1:32:A:ASP:H | 9        | 1.53          |
| (1,23)  | 1:30:A:SER:HG | 1:32:A:ASP:H | 14       | 1.53          |
| (2,40)  | 1:49:A:VAL:N  | 1:45:A:ARG:O | 5        | 1.51          |
| (2,39)  | 1:49:A:VAL:H  | 1:45:A:ARG:O | 14       | 1.51          |
| (1,23)  | 1:30:A:SER:HG | 1:32:A:ASP:H | 4        | 1.49          |
| (1,23)  | 1:30:A:SER:HG | 1:32:A:ASP:H | 11       | 1.46          |
| (1,23)  | 1:30:A:SER:HG | 1:32:A:ASP:H | 20       | 1.45          |
| (2,40)  | 1:49:A:VAL:N  | 1:45:A:ARG:O | 20       | 1.43          |
| (2,40)  | 1:49:A:VAL:N  | 1:45:A:ARG:O | 16       | 1.42          |
| (2,40)  | 1:49:A:VAL:N  | 1:45:A:ARG:O | 12       | 1.39          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (2,40)  | 1:49:A:VAL:N   | 1:45:A:ARG:O    | 17       | 1.39          |
| (2,40)  | 1:49:A:VAL:N   | 1:45:A:ARG:O    | 18       | 1.34          |
| (1,23)  | 1:30:A:SER:HG  | 1:32:A:ASP:H    | 5        | 1.32          |
| (1,115) | 1:47:A:LEU:H   | 1:49:A:VAL:H    | 2        | 1.29          |
| (2,39)  | 1:49:A:VAL:H   | 1:45:A:ARG:O    | 10       | 1.27          |
| (2,40)  | 1:49:A:VAL:N   | 1:45:A:ARG:O    | 3        | 1.24          |
| (2,39)  | 1:49:A:VAL:H   | 1:45:A:ARG:O    | 2        | 1.21          |
| (1,115) | 1:47:A:LEU:H   | 1:49:A:VAL:H    | 10       | 1.21          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD2  | 10       | 1.19          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD3  | 10       | 1.19          |
| (1,23)  | 1:30:A:SER:HG  | 1:32:A:ASP:H    | 6        | 1.18          |
| (1,23)  | 1:30:A:SER:HG  | 1:32:A:ASP:H    | 18       | 1.18          |
| (2,40)  | 1:49:A:VAL:N   | 1:45:A:ARG:O    | 13       | 1.14          |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD21 | 17       | 1.09          |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD22 | 17       | 1.09          |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD23 | 17       | 1.09          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD2  | 7        | 1.06          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD3  | 7        | 1.06          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD2  | 14       | 1.06          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD3  | 14       | 1.06          |
| (1,141) | 1:29:A:THR:HB  | 1:30:A:SER:H    | 12       | 1.02          |
| (1,141) | 1:29:A:THR:HB  | 1:30:A:SER:H    | 6        | 1.01          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD2  | 16       | 1.01          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD3  | 16       | 1.01          |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD21 | 14       | 1.0           |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD22 | 14       | 1.0           |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD23 | 14       | 1.0           |
| (1,23)  | 1:30:A:SER:HG  | 1:32:A:ASP:H    | 7        | 0.96          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD2  | 11       | 0.94          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD3  | 11       | 0.94          |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD21 | 20       | 0.93          |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD22 | 20       | 0.93          |
| (1,449) | 1:34:A:GLU:HB2 | 1:35:A:LEU:HD23 | 20       | 0.93          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD2  | 12       | 0.93          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD3  | 12       | 0.93          |
| (1,23)  | 1:30:A:SER:HG  | 1:32:A:ASP:H    | 10       | 0.92          |
| (2,40)  | 1:49:A:VAL:N   | 1:45:A:ARG:O    | 9        | 0.89          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD2  | 4        | 0.81          |
| (1,39)  | 1:12:A:LYS:H   | 1:12:A:LYS:HD3  | 4        | 0.81          |
| (1,586) | 1:44:A:HIS:HA  | 1:47:A:LEU:HG   | 16       | 0.79          |
| (1,586) | 1:44:A:HIS:HA  | 1:47:A:LEU:HG   | 11       | 0.78          |
| (1,586) | 1:44:A:HIS:HA  | 1:47:A:LEU:HG   | 19       | 0.78          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 20       | 0.78          |
| (1,279) | 1:44:A:HIS:HD2  | 1:45:A:ARG:H    | 9        | 0.78          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 7        | 0.77          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 18       | 0.77          |
| (1,279) | 1:44:A:HIS:HD2  | 1:45:A:ARG:H    | 15       | 0.77          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 1        | 0.75          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 1        | 0.75          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 1        | 0.75          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 8        | 0.72          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD21 | 9        | 0.72          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD22 | 9        | 0.72          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD23 | 9        | 0.72          |
| (1,115) | 1:47:A:LEU:H    | 1:49:A:VAL:H    | 8        | 0.72          |
| (2,39)  | 1:49:A:VAL:H    | 1:45:A:ARG:O    | 7        | 0.71          |
| (1,734) | 1:38:A:ALA:H    | 1:41:A:GLU:HG2  | 12       | 0.7           |
| (1,734) | 1:38:A:ALA:H    | 1:41:A:GLU:HG3  | 12       | 0.7           |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 7        | 0.7           |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 7        | 0.7           |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 7        | 0.7           |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 3        | 0.69          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD2  | 3        | 0.69          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD3  | 3        | 0.69          |
| (2,39)  | 1:49:A:VAL:H    | 1:45:A:ARG:O    | 8        | 0.68          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 12       | 0.68          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 4        | 0.68          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 4        | 0.68          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 4        | 0.68          |
| (2,40)  | 1:49:A:VAL:N    | 1:45:A:ARG:O    | 7        | 0.67          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 11       | 0.67          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 11       | 0.67          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 11       | 0.67          |
| (1,279) | 1:44:A:HIS:HD2  | 1:45:A:ARG:H    | 13       | 0.67          |
| (1,23)  | 1:30:A:SER:HG   | 1:32:A:ASP:H    | 1        | 0.67          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 4        | 0.66          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 4        | 0.66          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 4        | 0.66          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 2        | 0.65          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 2        | 0.65          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 2        | 0.65          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD11 | 1        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD12 | 1        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD13 | 1        | 0.64          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 6        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 6        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 6        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 7        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 7        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 7        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 9        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 9        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 9        | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 10       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 10       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 10       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 16       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 16       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 16       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 18       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 18       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 18       | 0.64          |
| (1,348) | 1:41:A:GLU:H   | 1:41:A:GLU:HG2  | 12       | 0.64          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 2        | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 2        | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 2        | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 3        | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 3        | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 3        | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 11       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 11       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 11       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 12       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 12       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 12       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 13       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 13       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 13       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 15       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 15       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 15       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD11 | 19       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD12 | 19       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2 | 1:35:A:LEU:HD13 | 19       | 0.63          |
| (1,316) | 1:18:A:TRP:HE1 | 1:23:A:LEU:HD21 | 13       | 0.63          |
| (1,316) | 1:18:A:TRP:HE1 | 1:23:A:LEU:HD22 | 13       | 0.63          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 13       | 0.63          |
| (1,279) | 1:44:A:HIS:HD2  | 1:45:A:ARG:H    | 19       | 0.63          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD11 | 8        | 0.62          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD12 | 8        | 0.62          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD13 | 8        | 0.62          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 11       | 0.62          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 11       | 0.62          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 11       | 0.62          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 16       | 0.61          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 16       | 0.61          |
| (2,40)  | 1:49:A:VAL:N    | 1:45:A:ARG:O    | 4        | 0.6           |
| (2,40)  | 1:49:A:VAL:N    | 1:45:A:ARG:O    | 19       | 0.6           |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 8        | 0.6           |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 5        | 0.6           |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD11 | 5        | 0.6           |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD12 | 5        | 0.6           |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD13 | 5        | 0.6           |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 15       | 0.6           |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 15       | 0.6           |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 15       | 0.6           |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 18       | 0.6           |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 18       | 0.6           |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 18       | 0.6           |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 2        | 0.59          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 2        | 0.59          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 2        | 0.59          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 12       | 0.59          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 12       | 0.59          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 12       | 0.59          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 4        | 0.58          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 4        | 0.58          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 4        | 0.58          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 11       | 0.58          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 11       | 0.58          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 10       | 0.58          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 10       | 0.58          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 10       | 0.58          |
| (1,279) | 1:44:A:HIS:HD2  | 1:45:A:ARG:H    | 11       | 0.57          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 19       | 0.57          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 19       | 0.57          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 19       | 0.57          |
| (2,40)  | 1:49:A:VAL:N    | 1:45:A:ARG:O    | 8        | 0.56          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,751) | 1:41:A:GLU:H    | 1:41:A:GLU:HG2  | 12       | 0.56          |
| (1,751) | 1:41:A:GLU:H    | 1:41:A:GLU:HG3  | 12       | 0.56          |
| (1,734) | 1:38:A:ALA:H    | 1:41:A:GLU:HG2  | 6        | 0.56          |
| (1,734) | 1:38:A:ALA:H    | 1:41:A:GLU:HG3  | 6        | 0.56          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 14       | 0.56          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 7        | 0.56          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 7        | 0.56          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 7        | 0.56          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 9        | 0.56          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 9        | 0.56          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 9        | 0.56          |
| (1,634) | 1:29:A:THR:H    | 1:30:A:SER:HB3  | 8        | 0.55          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 18       | 0.55          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 18       | 0.55          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 15       | 0.54          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 2        | 0.54          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 2        | 0.54          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 9        | 0.54          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 9        | 0.54          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 14       | 0.54          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 14       | 0.54          |
| (1,279) | 1:44:A:HIS:HD2  | 1:45:A:ARG:H    | 20       | 0.54          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 13       | 0.54          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 13       | 0.54          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 13       | 0.54          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 14       | 0.54          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 14       | 0.54          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 14       | 0.54          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 9        | 0.53          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 9        | 0.53          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 9        | 0.53          |
| (1,459) | 1:49:A:VAL:HG21 | 1:50:A:TYR:HD1  | 7        | 0.53          |
| (1,459) | 1:49:A:VAL:HG21 | 1:50:A:TYR:HD2  | 7        | 0.53          |
| (1,459) | 1:49:A:VAL:HG22 | 1:50:A:TYR:HD1  | 7        | 0.53          |
| (1,459) | 1:49:A:VAL:HG22 | 1:50:A:TYR:HD2  | 7        | 0.53          |
| (1,459) | 1:49:A:VAL:HG23 | 1:50:A:TYR:HD1  | 7        | 0.53          |
| (1,459) | 1:49:A:VAL:HG23 | 1:50:A:TYR:HD2  | 7        | 0.53          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 15       | 0.53          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 15       | 0.53          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 16       | 0.53          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 16       | 0.53          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 16       | 0.53          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 17       | 0.53          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 17       | 0.53          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 17       | 0.53          |
| (2,40)  | 1:49:A:VAL:N    | 1:45:A:ARG:O    | 1        | 0.52          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 17       | 0.52          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 17       | 0.52          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 17       | 0.52          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 7        | 0.52          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 7        | 0.52          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 12       | 0.52          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 12       | 0.52          |
| (1,21)  | 1:35:A:LEU:H    | 1:35:A:LEU:HG   | 17       | 0.52          |
| (2,39)  | 1:49:A:VAL:H    | 1:45:A:ARG:O    | 6        | 0.51          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 1        | 0.51          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 1        | 0.51          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 1        | 0.51          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 1        | 0.51          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 1        | 0.51          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 1        | 0.51          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 3        | 0.51          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 3        | 0.51          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 3        | 0.51          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 3        | 0.51          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 3        | 0.51          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 3        | 0.51          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 18       | 0.51          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 18       | 0.51          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 18       | 0.51          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 18       | 0.51          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 18       | 0.51          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 18       | 0.51          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 20       | 0.51          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 20       | 0.51          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 20       | 0.51          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 20       | 0.51          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 20       | 0.51          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 20       | 0.51          |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE1  | 12       | 0.51          |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE2  | 12       | 0.51          |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE1  | 12       | 0.51          |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE2  | 12       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG21 | 2        | 0.51          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG22 | 2        | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG23 | 2        | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG21 | 2        | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG22 | 2        | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG23 | 2        | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG21 | 7        | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG22 | 7        | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG23 | 7        | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG21 | 7        | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG22 | 7        | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG23 | 7        | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG21 | 12       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG22 | 12       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG23 | 12       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG21 | 12       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG22 | 12       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG23 | 12       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG21 | 13       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG22 | 13       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG23 | 13       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG21 | 13       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG22 | 13       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG23 | 13       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG21 | 14       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG22 | 14       | 0.51          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG23 | 14       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG21 | 14       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG22 | 14       | 0.51          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG23 | 14       | 0.51          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 5        | 0.51          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 5        | 0.51          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 6        | 0.51          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 6        | 0.51          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 9        | 0.51          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 9        | 0.51          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 17       | 0.51          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 17       | 0.51          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 7        | 0.51          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 7        | 0.51          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 7        | 0.51          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 2        | 0.51          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 2        | 0.51          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 2        | 0.51          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 4        | 0.51          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 4        | 0.51          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 4        | 0.51          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 20       | 0.51          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 20       | 0.51          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 4        | 0.51          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 4        | 0.51          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 1        | 0.51          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 2        | 0.51          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 3        | 0.51          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 10       | 0.51          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 12       | 0.51          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 13       | 0.51          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 15       | 0.51          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 18       | 0.51          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 18       | 0.51          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 6        | 0.51          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 6        | 0.51          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 6        | 0.51          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 8        | 0.51          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 8        | 0.51          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 8        | 0.51          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 13       | 0.51          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 13       | 0.51          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 13       | 0.51          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 16       | 0.51          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 20       | 0.51          |
| (1,165) | 1:3:A:LEU:H     | 1:4:A:GLY:H     | 16       | 0.51          |
| (1,743) | 1:39:A:CYS:HB2  | 1:40:A:ARG:HB2  | 8        | 0.5           |
| (1,743) | 1:39:A:CYS:HB2  | 1:40:A:ARG:HB3  | 8        | 0.5           |
| (1,743) | 1:39:A:CYS:HB3  | 1:40:A:ARG:HB2  | 8        | 0.5           |
| (1,743) | 1:39:A:CYS:HB3  | 1:40:A:ARG:HB3  | 8        | 0.5           |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 4        | 0.5           |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 4        | 0.5           |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 4        | 0.5           |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 4        | 0.5           |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 4        | 0.5           |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 4        | 0.5           |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE1  | 18       | 0.5           |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE2  | 18       | 0.5           |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE1  | 18       | 0.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE2  | 18       | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 1        | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 1        | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 4        | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 4        | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 10       | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 10       | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 16       | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 16       | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 20       | 0.5           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 20       | 0.5           |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 3        | 0.5           |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 3        | 0.5           |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 3        | 0.5           |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 14       | 0.5           |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 14       | 0.5           |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 14       | 0.5           |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 17       | 0.5           |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 18       | 0.5           |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 19       | 0.5           |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 19       | 0.5           |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 19       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 11       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 11       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 11       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 14       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 14       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 14       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 20       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 20       | 0.5           |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 20       | 0.5           |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 20       | 0.5           |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 20       | 0.5           |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 20       | 0.5           |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 20       | 0.5           |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 20       | 0.5           |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 20       | 0.5           |
| (1,414) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HA   | 2        | 0.5           |
| (1,414) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HA   | 2        | 0.5           |
| (1,414) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HA   | 4        | 0.5           |
| (1,414) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HA   | 4        | 0.5           |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 5        | 0.5           |

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| Key     | Atom-1          | Atom-2         | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H   | 6        | 0.5           |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H   | 8        | 0.5           |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H   | 9        | 0.5           |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H   | 11       | 0.5           |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H   | 16       | 0.5           |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H   | 17       | 0.5           |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H   | 19       | 0.5           |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H   | 20       | 0.5           |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE  | 14       | 0.5           |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H   | 5        | 0.5           |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H   | 5        | 0.5           |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H   | 5        | 0.5           |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H   | 9        | 0.5           |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H   | 9        | 0.5           |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H   | 9        | 0.5           |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H   | 10       | 0.5           |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H   | 10       | 0.5           |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H   | 10       | 0.5           |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H   | 11       | 0.5           |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H   | 11       | 0.5           |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H   | 11       | 0.5           |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H   | 14       | 0.5           |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H   | 14       | 0.5           |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H   | 14       | 0.5           |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H   | 16       | 0.5           |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H   | 16       | 0.5           |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H   | 16       | 0.5           |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H   | 17       | 0.5           |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H   | 17       | 0.5           |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H   | 17       | 0.5           |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H   | 6        | 0.5           |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H   | 6        | 0.5           |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H   | 6        | 0.5           |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H   | 5        | 0.5           |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H   | 5        | 0.5           |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H   | 5        | 0.5           |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2 | 1        | 0.5           |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2 | 3        | 0.5           |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2 | 4        | 0.5           |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2 | 6        | 0.5           |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2 | 8        | 0.5           |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2 | 12       | 0.5           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 18       | 0.5           |
| (1,182) | 1:25:A:ASP:HA   | 1:28:A:ASN:HD21 | 7        | 0.5           |
| (1,182) | 1:25:A:ASP:HA   | 1:28:A:ASN:HD21 | 18       | 0.5           |
| (1,165) | 1:3:A:LEU:H     | 1:4:A:GLY:H     | 4        | 0.5           |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 3        | 0.5           |
| (1,145) | 1:26:A:THR:HG21 | 1:30:A:SER:H    | 12       | 0.5           |
| (1,145) | 1:26:A:THR:HG22 | 1:30:A:SER:H    | 12       | 0.5           |
| (1,145) | 1:26:A:THR:HG23 | 1:30:A:SER:H    | 12       | 0.5           |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD2  | 15       | 0.5           |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD3  | 15       | 0.5           |
| (1,37)  | 1:11:A:LYS:HA   | 1:12:A:LYS:H    | 20       | 0.5           |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 17       | 0.5           |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE1  | 13       | 0.49          |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE2  | 13       | 0.49          |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE1  | 13       | 0.49          |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE2  | 13       | 0.49          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG21 | 18       | 0.49          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG22 | 18       | 0.49          |
| (1,711) | 1:24:A:ARG:HD2  | 1:27:A:ILE:HG23 | 18       | 0.49          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG21 | 18       | 0.49          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG22 | 18       | 0.49          |
| (1,711) | 1:24:A:ARG:HD3  | 1:27:A:ILE:HG23 | 18       | 0.49          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 11       | 0.49          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 11       | 0.49          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 4        | 0.49          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 12       | 0.49          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 10       | 0.49          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 14       | 0.49          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 14       | 0.49          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 14       | 0.49          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 14       | 0.49          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 14       | 0.49          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 14       | 0.49          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 16       | 0.49          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 16       | 0.49          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 16       | 0.49          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 16       | 0.49          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 16       | 0.49          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 16       | 0.49          |
| (1,321) | 1:12:A:LYS:H    | 1:12:A:LYS:HE2  | 4        | 0.49          |
| (1,321) | 1:12:A:LYS:H    | 1:12:A:LYS:HE3  | 4        | 0.49          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 7        | 0.49          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 14       | 0.49          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 20       | 0.49          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 3        | 0.49          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 3        | 0.49          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 3        | 0.49          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 13       | 0.49          |
| (1,145) | 1:26:A:THR:HG21 | 1:30:A:SER:H    | 6        | 0.49          |
| (1,145) | 1:26:A:THR:HG22 | 1:30:A:SER:H    | 6        | 0.49          |
| (1,145) | 1:26:A:THR:HG23 | 1:30:A:SER:H    | 6        | 0.49          |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD2  | 12       | 0.49          |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD3  | 12       | 0.49          |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD2  | 15       | 0.49          |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD3  | 15       | 0.49          |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 11       | 0.49          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 20       | 0.48          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 20       | 0.48          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 20       | 0.48          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 20       | 0.48          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 20       | 0.48          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 20       | 0.48          |
| (1,743) | 1:39:A:CYS:HB2  | 1:40:A:ARG:HB2  | 20       | 0.48          |
| (1,743) | 1:39:A:CYS:HB2  | 1:40:A:ARG:HB3  | 20       | 0.48          |
| (1,743) | 1:39:A:CYS:HB3  | 1:40:A:ARG:HB2  | 20       | 0.48          |
| (1,743) | 1:39:A:CYS:HB3  | 1:40:A:ARG:HB3  | 20       | 0.48          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 16       | 0.48          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 16       | 0.48          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 16       | 0.48          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 16       | 0.48          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 16       | 0.48          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 16       | 0.48          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD11 | 20       | 0.48          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD12 | 20       | 0.48          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD13 | 20       | 0.48          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 14       | 0.48          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 14       | 0.48          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 14       | 0.48          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 10       | 0.48          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 10       | 0.48          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 10       | 0.48          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 10       | 0.48          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 10       | 0.48          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 15       | 0.48          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 4        | 0.48          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 4        | 0.48          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 4        | 0.48          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 7        | 0.48          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 7        | 0.48          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 7        | 0.48          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 19       | 0.48          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 19       | 0.48          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 19       | 0.48          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 7        | 0.48          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 7        | 0.48          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 7        | 0.48          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 2        | 0.48          |
| (1,101) | 1:41:A:GLU:H    | 1:41:A:GLU:HG3  | 12       | 0.48          |
| (1,743) | 1:39:A:CYS:HB2  | 1:40:A:ARG:HB2  | 10       | 0.47          |
| (1,743) | 1:39:A:CYS:HB2  | 1:40:A:ARG:HB3  | 10       | 0.47          |
| (1,743) | 1:39:A:CYS:HB3  | 1:40:A:ARG:HB2  | 10       | 0.47          |
| (1,743) | 1:39:A:CYS:HB3  | 1:40:A:ARG:HB3  | 10       | 0.47          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 17       | 0.47          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 17       | 0.47          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 17       | 0.47          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 3        | 0.47          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 3        | 0.47          |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 4        | 0.47          |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 17       | 0.47          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 15       | 0.47          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD2  | 20       | 0.47          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD3  | 20       | 0.47          |
| (1,26)  | 1:10:A:THR:HA   | 1:11:A:LYS:H    | 8        | 0.47          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG11 | 18       | 0.46          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG12 | 18       | 0.46          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG13 | 18       | 0.46          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG21 | 18       | 0.46          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG22 | 18       | 0.46          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG23 | 18       | 0.46          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 2        | 0.46          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 2        | 0.46          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 2        | 0.46          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 2        | 0.46          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 2        | 0.46          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 2        | 0.46          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 15       | 0.46          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 15       | 0.46          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 15       | 0.46          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 15       | 0.46          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 15       | 0.46          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 15       | 0.46          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD11 | 4        | 0.46          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD12 | 4        | 0.46          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD13 | 4        | 0.46          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 6        | 0.46          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 6        | 0.46          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 6        | 0.46          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 6        | 0.46          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 6        | 0.46          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 6        | 0.46          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 6        | 0.46          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 6        | 0.46          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 6        | 0.46          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 9        | 0.46          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 9        | 0.46          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 9        | 0.46          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 9        | 0.46          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 9        | 0.46          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 9        | 0.46          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 10       | 0.46          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 10       | 0.46          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 2        | 0.46          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 2        | 0.46          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 2        | 0.46          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 14       | 0.46          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 17       | 0.46          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 6        | 0.46          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 19       | 0.45          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 19       | 0.45          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 19       | 0.45          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 19       | 0.45          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 19       | 0.45          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 19       | 0.45          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 14       | 0.45          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 7        | 0.45          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 7        | 0.45          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 7        | 0.45          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 12       | 0.45          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 12       | 0.45          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 12       | 0.45          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD21 | 16       | 0.45          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD22 | 16       | 0.45          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD23 | 16       | 0.45          |
| (1,414) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HA   | 7        | 0.45          |
| (1,414) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HA   | 7        | 0.45          |
| (1,664) | 1:12:A:LYS:HB2  | 1:13:A:TYR:H    | 20       | 0.44          |
| (1,664) | 1:12:A:LYS:HB3  | 1:13:A:TYR:H    | 20       | 0.44          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 8        | 0.44          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 8        | 0.44          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 19       | 0.44          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 19       | 0.44          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 7        | 0.44          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 14       | 0.44          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 14       | 0.44          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 14       | 0.44          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD11 | 14       | 0.44          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD12 | 14       | 0.44          |
| (1,512) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD13 | 14       | 0.44          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 1        | 0.44          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 1        | 0.44          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 1        | 0.44          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 2        | 0.44          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 2        | 0.44          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 2        | 0.44          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 20       | 0.44          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 20       | 0.44          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 20       | 0.44          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 9        | 0.44          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 9        | 0.44          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 9        | 0.44          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 19       | 0.44          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 4        | 0.44          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 17       | 0.44          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 6        | 0.43          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 6        | 0.43          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 6        | 0.43          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 18       | 0.43          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 18       | 0.43          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 18       | 0.43          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 20       | 0.43          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 20       | 0.43          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 20       | 0.43          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 18       | 0.43          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 18       | 0.43          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 20       | 0.43          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 20       | 0.43          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 20       | 0.43          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 12       | 0.43          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 12       | 0.43          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 12       | 0.43          |
| (1,185) | 1:26:A:THR:HG1  | 1:27:A:ILE:H    | 20       | 0.43          |
| (1,182) | 1:25:A:ASP:HA   | 1:28:A:ASN:HD21 | 13       | 0.43          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG11 | 20       | 0.42          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG12 | 20       | 0.42          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG13 | 20       | 0.42          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG21 | 20       | 0.42          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG22 | 20       | 0.42          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG23 | 20       | 0.42          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 17       | 0.42          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 17       | 0.42          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 17       | 0.42          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 17       | 0.42          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 17       | 0.42          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 17       | 0.42          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 15       | 0.42          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 15       | 0.42          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 15       | 0.42          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 19       | 0.42          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 17       | 0.42          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 17       | 0.42          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 17       | 0.42          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD21 | 6        | 0.42          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD22 | 6        | 0.42          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD23 | 6        | 0.42          |
| (1,330) | 1:20:A:TYR:HE1  | 1:24:A:ARG:HD2  | 6        | 0.42          |
| (1,330) | 1:20:A:TYR:HE2  | 1:24:A:ARG:HD2  | 6        | 0.42          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 14       | 0.42          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 14       | 0.42          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 14       | 0.42          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 14       | 0.42          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 14       | 0.42          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 14       | 0.42          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 17       | 0.42          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 17       | 0.42          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 17       | 0.42          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 8        | 0.42          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 8        | 0.42          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 8        | 0.42          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 11       | 0.42          |
| (1,170) | 1:28:A:ASN:HB2  | 1:30:A:SER:H    | 4        | 0.42          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 7        | 0.42          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 20       | 0.42          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 1        | 0.42          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 11       | 0.42          |
| (1,115) | 1:47:A:LEU:H    | 1:49:A:VAL:H    | 7        | 0.42          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD2  | 9        | 0.42          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD3  | 9        | 0.42          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD2  | 18       | 0.42          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD3  | 18       | 0.42          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 20       | 0.41          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 20       | 0.41          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 20       | 0.41          |
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 14       | 0.41          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 12       | 0.41          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 16       | 0.41          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 16       | 0.41          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 16       | 0.41          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 4        | 0.41          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 4        | 0.41          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 4        | 0.41          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 10       | 0.41          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 6        | 0.41          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 14       | 0.41          |
| (1,734) | 1:38:A:ALA:H    | 1:41:A:GLU:HG2  | 10       | 0.4           |
| (1,734) | 1:38:A:ALA:H    | 1:41:A:GLU:HG3  | 10       | 0.4           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 3        | 0.4           |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 3        | 0.4           |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 13       | 0.4           |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 13       | 0.4           |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 13       | 0.4           |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 12       | 0.4           |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 12       | 0.4           |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 12       | 0.4           |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 18       | 0.4           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 18       | 0.4           |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 18       | 0.4           |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 1        | 0.4           |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 1        | 0.4           |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 13       | 0.4           |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 13       | 0.4           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 12       | 0.4           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 12       | 0.4           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 12       | 0.4           |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 8        | 0.4           |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 12       | 0.4           |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 12       | 0.4           |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 12       | 0.4           |
| (1,185) | 1:26:A:THR:HG1  | 1:27:A:ILE:H    | 12       | 0.4           |
| (1,170) | 1:28:A:ASN:HB2  | 1:30:A:SER:H    | 3        | 0.4           |
| (1,170) | 1:28:A:ASN:HB2  | 1:30:A:SER:H    | 8        | 0.4           |
| (1,165) | 1:3:A:LEU:H     | 1:4:A:GLY:H     | 9        | 0.4           |
| (1,165) | 1:3:A:LEU:H     | 1:4:A:GLY:H     | 13       | 0.4           |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE1  | 11       | 0.39          |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE2  | 11       | 0.39          |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE1  | 11       | 0.39          |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE2  | 11       | 0.39          |
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 3        | 0.39          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 9        | 0.39          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 8        | 0.39          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 8        | 0.39          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 8        | 0.39          |
| (1,534) | 1:44:A:HIS:HA   | 1:44:A:HIS:HD2  | 3        | 0.39          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 3        | 0.39          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 3        | 0.39          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 3        | 0.39          |
| (1,225) | 1:31:A:CYS:H    | 1:35:A:LEU:HD11 | 3        | 0.39          |
| (1,225) | 1:31:A:CYS:H    | 1:35:A:LEU:HD12 | 3        | 0.39          |
| (1,225) | 1:31:A:CYS:H    | 1:35:A:LEU:HD13 | 3        | 0.39          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 7        | 0.39          |
| (1,185) | 1:26:A:THR:HG1  | 1:27:A:ILE:H    | 7        | 0.39          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 4        | 0.39          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD2  | 2        | 0.39          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD3  | 2        | 0.39          |
| (1,805) | 1:49:A:VAL:HG11 | 1:51:A:HIS:H    | 17       | 0.38          |
| (1,805) | 1:49:A:VAL:HG12 | 1:51:A:HIS:H    | 17       | 0.38          |
| (1,805) | 1:49:A:VAL:HG13 | 1:51:A:HIS:H    | 17       | 0.38          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,805) | 1:49:A:VAL:HG21 | 1:51:A:HIS:H    | 17       | 0.38          |
| (1,805) | 1:49:A:VAL:HG22 | 1:51:A:HIS:H    | 17       | 0.38          |
| (1,805) | 1:49:A:VAL:HG23 | 1:51:A:HIS:H    | 17       | 0.38          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 14       | 0.38          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 14       | 0.38          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 14       | 0.38          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 14       | 0.38          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 14       | 0.38          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 14       | 0.38          |
| (1,595) | 1:24:A:ARG:HA   | 1:24:A:ARG:HD3  | 2        | 0.38          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 16       | 0.38          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 16       | 0.38          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 16       | 0.38          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 12       | 0.38          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 12       | 0.38          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 12       | 0.38          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 12       | 0.38          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 12       | 0.38          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 12       | 0.38          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 20       | 0.38          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 20       | 0.38          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 20       | 0.38          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD2  | 13       | 0.38          |
| (1,425) | 1:12:A:LYS:HA   | 1:12:A:LYS:HD3  | 13       | 0.38          |
| (1,379) | 1:45:A:ARG:H    | 1:45:A:ARG:HG3  | 19       | 0.38          |
| (1,379) | 1:45:A:ARG:H    | 1:45:A:ARG:HG3  | 20       | 0.38          |
| (1,330) | 1:20:A:TYR:HE1  | 1:24:A:ARG:HD2  | 17       | 0.38          |
| (1,330) | 1:20:A:TYR:HE2  | 1:24:A:ARG:HD2  | 17       | 0.38          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 3        | 0.38          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 15       | 0.38          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 15       | 0.38          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 15       | 0.38          |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 19       | 0.38          |
| (1,185) | 1:26:A:THR:HG1  | 1:27:A:ILE:H    | 6        | 0.38          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 8        | 0.38          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 18       | 0.38          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 19       | 0.38          |
| (1,89)  | 1:45:A:ARG:H    | 1:45:A:ARG:HG2  | 2        | 0.38          |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 18       | 0.37          |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 18       | 0.37          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 12       | 0.37          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 12       | 0.37          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 2        | 0.37          |
| (1,595) | 1:24:A:ARG:HA   | 1:24:A:ARG:HD3  | 7        | 0.37          |
| (1,595) | 1:24:A:ARG:HA   | 1:24:A:ARG:HD3  | 18       | 0.37          |
| (1,489) | 1:26:A:THR:HA   | 1:30:A:SER:HB3  | 8        | 0.37          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 20       | 0.37          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 20       | 0.37          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 20       | 0.37          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 17       | 0.37          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 17       | 0.37          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 17       | 0.37          |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 1        | 0.37          |
| (1,182) | 1:25:A:ASP:HA   | 1:28:A:ASN:HD21 | 20       | 0.37          |
| (1,12)  | 1:51:A:HIS:H    | 1:51:A:HIS:HD2  | 8        | 0.37          |
| (1,805) | 1:49:A:VAL:HG11 | 1:51:A:HIS:H    | 11       | 0.36          |
| (1,805) | 1:49:A:VAL:HG12 | 1:51:A:HIS:H    | 11       | 0.36          |
| (1,805) | 1:49:A:VAL:HG13 | 1:51:A:HIS:H    | 11       | 0.36          |
| (1,805) | 1:49:A:VAL:HG21 | 1:51:A:HIS:H    | 11       | 0.36          |
| (1,805) | 1:49:A:VAL:HG22 | 1:51:A:HIS:H    | 11       | 0.36          |
| (1,805) | 1:49:A:VAL:HG23 | 1:51:A:HIS:H    | 11       | 0.36          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG11 | 10       | 0.36          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG12 | 10       | 0.36          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG13 | 10       | 0.36          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG21 | 10       | 0.36          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG22 | 10       | 0.36          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG23 | 10       | 0.36          |
| (1,684) | 1:19:A:LYS:H    | 1:19:A:LYS:HG2  | 16       | 0.36          |
| (1,684) | 1:19:A:LYS:H    | 1:19:A:LYS:HG3  | 16       | 0.36          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 6        | 0.36          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 11       | 0.36          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD11 | 12       | 0.36          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD12 | 12       | 0.36          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD13 | 12       | 0.36          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD11 | 12       | 0.36          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD12 | 12       | 0.36          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD13 | 12       | 0.36          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD11 | 12       | 0.36          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD12 | 12       | 0.36          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD13 | 12       | 0.36          |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB2  | 3        | 0.36          |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB3  | 3        | 0.36          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 19       | 0.36          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 19       | 0.36          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 19       | 0.36          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 3        | 0.36          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 20       | 0.36          |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 7        | 0.36          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 14       | 0.35          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 14       | 0.35          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 14       | 0.35          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 14       | 0.35          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 14       | 0.35          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 14       | 0.35          |
| (1,664) | 1:12:A:LYS:HB2  | 1:13:A:TYR:H    | 14       | 0.35          |
| (1,664) | 1:12:A:LYS:HB3  | 1:13:A:TYR:H    | 14       | 0.35          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 17       | 0.35          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 15       | 0.35          |
| (1,534) | 1:44:A:HIS:HA   | 1:44:A:HIS:HD2  | 10       | 0.35          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 17       | 0.35          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 17       | 0.35          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 17       | 0.35          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 17       | 0.35          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 17       | 0.35          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 17       | 0.35          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 2        | 0.35          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 5        | 0.35          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 14       | 0.35          |
| (1,289) | 1:27:A:ILE:HG13 | 1:28:A:ASN:HD21 | 2        | 0.35          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 7        | 0.35          |
| (1,12)  | 1:51:A:HIS:H    | 1:51:A:HIS:HD2  | 7        | 0.35          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG11 | 10       | 0.34          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG12 | 10       | 0.34          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG13 | 10       | 0.34          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG21 | 10       | 0.34          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG22 | 10       | 0.34          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG23 | 10       | 0.34          |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE1  | 14       | 0.34          |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE2  | 14       | 0.34          |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE1  | 14       | 0.34          |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE2  | 14       | 0.34          |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 7        | 0.34          |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 7        | 0.34          |
| (1,664) | 1:12:A:LYS:HB2  | 1:13:A:TYR:H    | 10       | 0.34          |
| (1,664) | 1:12:A:LYS:HB3  | 1:13:A:TYR:H    | 10       | 0.34          |
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 15       | 0.34          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 20       | 0.34          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 1        | 0.34          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 1        | 0.34          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 1        | 0.34          |
| (1,544) | 1:32:A:ASP:HB3  | 1:35:A:LEU:HG   | 17       | 0.34          |
| (1,534) | 1:44:A:HIS:HA   | 1:44:A:HIS:HD2  | 16       | 0.34          |
| (1,444) | 1:26:A:THR:HG21 | 1:35:A:LEU:HD11 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG21 | 1:35:A:LEU:HD12 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG21 | 1:35:A:LEU:HD13 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG22 | 1:35:A:LEU:HD11 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG22 | 1:35:A:LEU:HD12 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG22 | 1:35:A:LEU:HD13 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG23 | 1:35:A:LEU:HD11 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG23 | 1:35:A:LEU:HD12 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG23 | 1:35:A:LEU:HD13 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG21 | 1:35:A:LEU:HD21 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG21 | 1:35:A:LEU:HD22 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG21 | 1:35:A:LEU:HD23 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG22 | 1:35:A:LEU:HD21 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG22 | 1:35:A:LEU:HD22 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG22 | 1:35:A:LEU:HD23 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG23 | 1:35:A:LEU:HD21 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG23 | 1:35:A:LEU:HD22 | 7        | 0.34          |
| (1,444) | 1:26:A:THR:HG23 | 1:35:A:LEU:HD23 | 7        | 0.34          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 11       | 0.34          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 11       | 0.34          |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 19       | 0.34          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 12       | 0.34          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 17       | 0.34          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 15       | 0.34          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 15       | 0.34          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 15       | 0.34          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 7        | 0.34          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 9        | 0.34          |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 8        | 0.34          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 7        | 0.34          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 12       | 0.34          |
| (1,162) | 1:10:A:THR:H    | 1:10:A:THR:HB   | 19       | 0.34          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 10       | 0.34          |
| (1,89)  | 1:45:A:ARG:H    | 1:45:A:ARG:HG2  | 15       | 0.34          |
| (1,37)  | 1:11:A:LYS:HA   | 1:12:A:LYS:H    | 14       | 0.34          |
| (1,745) | 1:40:A:ARG:H    | 1:40:A:ARG:HG2  | 2        | 0.33          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,745) | 1:40:A:ARG:H    | 1:40:A:ARG:HG3  | 2        | 0.33          |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 10       | 0.33          |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 10       | 0.33          |
| (1,664) | 1:12:A:LYS:HB2  | 1:13:A:TYR:H    | 2        | 0.33          |
| (1,664) | 1:12:A:LYS:HB3  | 1:13:A:TYR:H    | 2        | 0.33          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 6        | 0.33          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 6        | 0.33          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 6        | 0.33          |
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 18       | 0.33          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 4        | 0.33          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 4        | 0.33          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 4        | 0.33          |
| (1,536) | 1:20:A:TYR:HE1  | 1:24:A:ARG:HD3  | 5        | 0.33          |
| (1,536) | 1:20:A:TYR:HE2  | 1:24:A:ARG:HD3  | 5        | 0.33          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 6        | 0.33          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 15       | 0.33          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 15       | 0.33          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 15       | 0.33          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 16       | 0.33          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 16       | 0.33          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 16       | 0.33          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 4        | 0.33          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 4        | 0.33          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 4        | 0.33          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 8        | 0.33          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 8        | 0.33          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 8        | 0.33          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 6        | 0.33          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 6        | 0.33          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 6        | 0.33          |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 9        | 0.33          |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 20       | 0.33          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 8        | 0.33          |
| (1,185) | 1:26:A:THR:HG1  | 1:27:A:ILE:H    | 18       | 0.33          |
| (1,171) | 1:30:A:SER:H    | 1:30:A:SER:HG   | 12       | 0.33          |
| (1,21)  | 1:35:A:LEU:H    | 1:35:A:LEU:HG   | 20       | 0.33          |
| (1,13)  | 1:50:A:TYR:HA   | 1:51:A:HIS:H    | 20       | 0.33          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG11 | 13       | 0.32          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG12 | 13       | 0.32          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG13 | 13       | 0.32          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG21 | 13       | 0.32          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG22 | 13       | 0.32          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG23 | 13       | 0.32          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 3        | 0.32          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 9        | 0.32          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 9        | 0.32          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 9        | 0.32          |
| (1,439) | 1:18:A:TRP:HZ3  | 1:26:A:THR:HG21 | 20       | 0.32          |
| (1,439) | 1:18:A:TRP:HZ3  | 1:26:A:THR:HG22 | 20       | 0.32          |
| (1,439) | 1:18:A:TRP:HZ3  | 1:26:A:THR:HG23 | 20       | 0.32          |
| (1,414) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HA   | 20       | 0.32          |
| (1,414) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HA   | 20       | 0.32          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD11 | 13       | 0.32          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD12 | 13       | 0.32          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD13 | 13       | 0.32          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 8        | 0.32          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 8        | 0.32          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 8        | 0.32          |
| (1,302) | 1:15:A:LEU:H    | 1:17:A:LYS:H    | 4        | 0.32          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 3        | 0.32          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 3        | 0.32          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 3        | 0.32          |
| (1,241) | 1:13:A:TYR:HE1  | 1:35:A:LEU:H    | 20       | 0.32          |
| (1,241) | 1:13:A:TYR:HE2  | 1:35:A:LEU:H    | 20       | 0.32          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 8        | 0.32          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 12       | 0.32          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 5        | 0.32          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 6        | 0.32          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 6        | 0.32          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 6        | 0.32          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 16       | 0.32          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 16       | 0.32          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 16       | 0.32          |
| (1,162) | 1:10:A:THR:H    | 1:10:A:THR:HB   | 7        | 0.32          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 5        | 0.32          |
| (1,143) | 1:26:A:THR:HA   | 1:30:A:SER:H    | 6        | 0.32          |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD2  | 13       | 0.32          |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD3  | 13       | 0.32          |
| (1,37)  | 1:11:A:LYS:HA   | 1:12:A:LYS:H    | 7        | 0.32          |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 5        | 0.32          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 7        | 0.31          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 11       | 0.31          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 18       | 0.31          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 17       | 0.31          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 7        | 0.31          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 14       | 0.31          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 20       | 0.31          |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 8        | 0.31          |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 12       | 0.31          |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 17       | 0.31          |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 18       | 0.31          |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 19       | 0.31          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG11 | 20       | 0.31          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG12 | 20       | 0.31          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG13 | 20       | 0.31          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG21 | 20       | 0.31          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG22 | 20       | 0.31          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG23 | 20       | 0.31          |
| (1,731) | 1:37:A:ALA:HA   | 1:40:A:ARG:HD2  | 12       | 0.31          |
| (1,731) | 1:37:A:ALA:HA   | 1:40:A:ARG:HD3  | 12       | 0.31          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 5        | 0.31          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 5        | 0.31          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 5        | 0.31          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 5        | 0.31          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 5        | 0.31          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 5        | 0.31          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 11       | 0.31          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 11       | 0.31          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 11       | 0.31          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 11       | 0.31          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 11       | 0.31          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 11       | 0.31          |
| (1,664) | 1:12:A:LYS:HB2  | 1:13:A:TYR:H    | 18       | 0.31          |
| (1,664) | 1:12:A:LYS:HB3  | 1:13:A:TYR:H    | 18       | 0.31          |
| (1,595) | 1:24:A:ARG:HA   | 1:24:A:ARG:HD3  | 14       | 0.31          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 10       | 0.31          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 10       | 0.31          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 10       | 0.31          |
| (1,544) | 1:32:A:ASP:HB3  | 1:35:A:LEU:HG   | 20       | 0.31          |
| (1,392) | 1:18:A:TRP:HZ3  | 1:23:A:LEU:HA   | 17       | 0.31          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 14       | 0.31          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 14       | 0.31          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 18       | 0.31          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 18       | 0.31          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 18       | 0.31          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 6        | 0.31          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,185) | 1:26:A:THR:HG1 | 1:27:A:ILE:H    | 2        | 0.31          |
| (1,185) | 1:26:A:THR:HG1 | 1:27:A:ILE:H    | 10       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD21 | 7        | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD22 | 7        | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD23 | 7        | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD21 | 11       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD22 | 11       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD23 | 11       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD21 | 12       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD22 | 12       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD23 | 12       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD21 | 13       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD22 | 13       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD23 | 13       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD21 | 18       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD22 | 18       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD23 | 18       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD21 | 19       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD22 | 19       | 0.31          |
| (1,172) | 1:29:A:THR:H   | 1:36:A:LEU:HD23 | 19       | 0.31          |
| (1,162) | 1:10:A:THR:H   | 1:10:A:THR:HB   | 8        | 0.31          |
| (1,110) | 1:49:A:VAL:H   | 1:49:A:VAL:HB   | 9        | 0.31          |
| (1,21)  | 1:35:A:LEU:H   | 1:35:A:LEU:HG   | 14       | 0.31          |
| (1,13)  | 1:50:A:TYR:HA  | 1:51:A:HIS:H    | 6        | 0.31          |
| (2,37)  | 1:48:A:LYS:H   | 1:44:A:HIS:O    | 2        | 0.3           |
| (2,37)  | 1:48:A:LYS:H   | 1:44:A:HIS:O    | 9        | 0.3           |
| (2,37)  | 1:48:A:LYS:H   | 1:44:A:HIS:O    | 10       | 0.3           |
| (2,33)  | 1:45:A:ARG:H   | 1:41:A:GLU:O    | 3        | 0.3           |
| (2,33)  | 1:45:A:ARG:H   | 1:41:A:GLU:O    | 4        | 0.3           |
| (2,33)  | 1:45:A:ARG:H   | 1:41:A:GLU:O    | 14       | 0.3           |
| (2,31)  | 1:44:A:HIS:H   | 1:40:A:ARG:O    | 6        | 0.3           |
| (2,27)  | 1:42:A:GLU:H   | 1:38:A:ALA:O    | 1        | 0.3           |
| (2,27)  | 1:42:A:GLU:H   | 1:38:A:ALA:O    | 4        | 0.3           |
| (2,27)  | 1:42:A:GLU:H   | 1:38:A:ALA:O    | 10       | 0.3           |
| (2,27)  | 1:42:A:GLU:H   | 1:38:A:ALA:O    | 18       | 0.3           |
| (2,25)  | 1:41:A:GLU:H   | 1:37:A:ALA:O    | 11       | 0.3           |
| (2,25)  | 1:41:A:GLU:H   | 1:37:A:ALA:O    | 17       | 0.3           |
| (2,25)  | 1:41:A:GLU:H   | 1:37:A:ALA:O    | 20       | 0.3           |
| (2,23)  | 1:40:A:ARG:H   | 1:36:A:LEU:O    | 8        | 0.3           |
| (2,17)  | 1:37:A:ALA:H   | 1:33:A:ILE:O    | 1        | 0.3           |
| (2,17)  | 1:37:A:ALA:H   | 1:33:A:ILE:O    | 2        | 0.3           |
| (2,17)  | 1:37:A:ALA:H   | 1:33:A:ILE:O    | 3        | 0.3           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 4        | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 5        | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 6        | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 7        | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 9        | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 10       | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 11       | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 13       | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 14       | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 15       | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 16       | 0.3           |
| (2,17)  | 1:37:A:ALA:H    | 1:33:A:ILE:O    | 20       | 0.3           |
| (2,13)  | 1:29:A:THR:H    | 1:25:A:ASP:O    | 3        | 0.3           |
| (2,13)  | 1:29:A:THR:H    | 1:25:A:ASP:O    | 4        | 0.3           |
| (2,13)  | 1:29:A:THR:H    | 1:25:A:ASP:O    | 8        | 0.3           |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 16       | 0.3           |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 17       | 0.3           |
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 12       | 0.3           |
| (2,5)   | 1:25:A:ASP:H    | 1:21:A:ALA:O    | 17       | 0.3           |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 7        | 0.3           |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 7        | 0.3           |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 7        | 0.3           |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 7        | 0.3           |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 7        | 0.3           |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 7        | 0.3           |
| (1,661) | 1:12:A:LYS:H    | 1:12:A:LYS:HB2  | 5        | 0.3           |
| (1,661) | 1:12:A:LYS:H    | 1:12:A:LYS:HB3  | 5        | 0.3           |
| (1,595) | 1:24:A:ARG:HA   | 1:24:A:ARG:HD3  | 12       | 0.3           |
| (1,595) | 1:24:A:ARG:HA   | 1:24:A:ARG:HD3  | 13       | 0.3           |
| (1,463) | 1:15:A:LEU:HD21 | 1:18:A:TRP:HE3  | 19       | 0.3           |
| (1,463) | 1:15:A:LEU:HD22 | 1:18:A:TRP:HE3  | 19       | 0.3           |
| (1,463) | 1:15:A:LEU:HD23 | 1:18:A:TRP:HE3  | 19       | 0.3           |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD21 | 19       | 0.3           |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD22 | 19       | 0.3           |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD23 | 19       | 0.3           |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB2  | 1        | 0.3           |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB3  | 1        | 0.3           |
| (1,361) | 1:49:A:VAL:HA   | 1:50:A:TYR:H    | 5        | 0.3           |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB1  | 11       | 0.3           |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB2  | 11       | 0.3           |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB3  | 11       | 0.3           |
| (1,330) | 1:20:A:TYR:HE1  | 1:24:A:ARG:HD2  | 8        | 0.3           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,330) | 1:20:A:TYR:HE2  | 1:24:A:ARG:HD2  | 8        | 0.3           |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 8        | 0.3           |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 8        | 0.3           |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 8        | 0.3           |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 7        | 0.3           |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 7        | 0.3           |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 7        | 0.3           |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 5        | 0.3           |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 5        | 0.3           |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 5        | 0.3           |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 14       | 0.3           |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 17       | 0.3           |
| (1,185) | 1:26:A:THR:HG1  | 1:27:A:ILE:H    | 14       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 9        | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 9        | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 9        | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 10       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 10       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 10       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 14       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 14       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 14       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 20       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 20       | 0.3           |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 20       | 0.3           |
| (1,110) | 1:49:A:VAL:H    | 1:49:A:VAL:HB   | 3        | 0.3           |
| (1,110) | 1:49:A:VAL:H    | 1:49:A:VAL:HB   | 15       | 0.3           |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 18       | 0.29          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 20       | 0.29          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 2        | 0.29          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 14       | 0.29          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 8        | 0.29          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 5        | 0.29          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 14       | 0.29          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 4        | 0.29          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 6        | 0.29          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 18       | 0.29          |
| (2,5)   | 1:25:A:ASP:H    | 1:21:A:ALA:O    | 19       | 0.29          |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 7        | 0.29          |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE1  | 1        | 0.29          |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE2  | 1        | 0.29          |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE1  | 1        | 0.29          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE2  | 1        | 0.29          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 19       | 0.29          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 19       | 0.29          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 19       | 0.29          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 18       | 0.29          |
| (1,569) | 1:15:A:LEU:HG   | 1:38:A:ALA:HB1  | 14       | 0.29          |
| (1,569) | 1:15:A:LEU:HG   | 1:38:A:ALA:HB2  | 14       | 0.29          |
| (1,569) | 1:15:A:LEU:HG   | 1:38:A:ALA:HB3  | 14       | 0.29          |
| (1,431) | 1:21:A:ALA:HA   | 1:24:A:ARG:HB2  | 7        | 0.29          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 13       | 0.29          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 18       | 0.29          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 11       | 0.29          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 7        | 0.29          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 7        | 0.29          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 7        | 0.29          |
| (1,254) | 1:15:A:LEU:HD11 | 1:39:A:CYS:H    | 14       | 0.29          |
| (1,254) | 1:15:A:LEU:HD12 | 1:39:A:CYS:H    | 14       | 0.29          |
| (1,254) | 1:15:A:LEU:HD13 | 1:39:A:CYS:H    | 14       | 0.29          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 2        | 0.29          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 15       | 0.29          |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 14       | 0.29          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 5        | 0.29          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 5        | 0.29          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 5        | 0.29          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 9        | 0.29          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 14       | 0.28          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 2        | 0.28          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 10       | 0.28          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 4        | 0.28          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 5        | 0.28          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 13       | 0.28          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 19       | 0.28          |
| (2,23)  | 1:40:A:ARG:H    | 1:36:A:LEU:O    | 4        | 0.28          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 1        | 0.28          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 5        | 0.28          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 11       | 0.28          |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 17       | 0.28          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 3        | 0.28          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 11       | 0.28          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 11       | 0.28          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 11       | 0.28          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 14       | 0.28          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 17       | 0.28          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 8        | 0.28          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 8        | 0.28          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 8        | 0.28          |
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD21 | 4        | 0.28          |
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD22 | 4        | 0.28          |
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD23 | 4        | 0.28          |
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD21 | 4        | 0.28          |
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD22 | 4        | 0.28          |
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD23 | 4        | 0.28          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 17       | 0.28          |
| (1,361) | 1:49:A:VAL:HA   | 1:50:A:TYR:H    | 7        | 0.28          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 10       | 0.28          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 10       | 0.28          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 10       | 0.28          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 17       | 0.28          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 2        | 0.28          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 2        | 0.28          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 6        | 0.28          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 6        | 0.28          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 18       | 0.28          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 18       | 0.28          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 18       | 0.28          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 11       | 0.28          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 11       | 0.28          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 11       | 0.28          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 16       | 0.28          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 16       | 0.28          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 16       | 0.28          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 18       | 0.28          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 20       | 0.28          |
| (1,143) | 1:26:A:THR:HA   | 1:30:A:SER:H    | 12       | 0.28          |
| (1,23)  | 1:30:A:SER:HG   | 1:32:A:ASP:H    | 16       | 0.28          |
| (1,13)  | 1:50:A:TYR:HA   | 1:51:A:HIS:H    | 13       | 0.28          |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 12       | 0.28          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 4        | 0.27          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 7        | 0.27          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 11       | 0.27          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 8        | 0.27          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 12       | 0.27          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 4        | 0.27          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 7        | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 14       | 0.27          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 18       | 0.27          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 15       | 0.27          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 8        | 0.27          |
| (2,4)   | 1:24:A:ARG:N    | 1:20:A:TYR:O    | 7        | 0.27          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 12       | 0.27          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 12       | 0.27          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 12       | 0.27          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 12       | 0.27          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 12       | 0.27          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 12       | 0.27          |
| (1,661) | 1:12:A:LYS:H    | 1:12:A:LYS:HB2  | 12       | 0.27          |
| (1,661) | 1:12:A:LYS:H    | 1:12:A:LYS:HB3  | 12       | 0.27          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 13       | 0.27          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 13       | 0.27          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 16       | 0.27          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 16       | 0.27          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 16       | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 1        | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 1        | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 1        | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 10       | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 10       | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 10       | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 20       | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 20       | 0.27          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 20       | 0.27          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 19       | 0.27          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 19       | 0.27          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 19       | 0.27          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD21 | 13       | 0.27          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD22 | 13       | 0.27          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD23 | 13       | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 3        | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 5        | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 7        | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 8        | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 11       | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 12       | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 15       | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 19       | 0.27          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 20       | 0.27          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,375) | 1:40:A:ARG:H    | 1:40:A:ARG:HG2  | 2        | 0.27          |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB2  | 2        | 0.27          |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB3  | 2        | 0.27          |
| (1,324) | 1:27:A:ILE:HD11 | 1:43:A:PHE:HD1  | 12       | 0.27          |
| (1,324) | 1:27:A:ILE:HD11 | 1:43:A:PHE:HD2  | 12       | 0.27          |
| (1,324) | 1:27:A:ILE:HD12 | 1:43:A:PHE:HD1  | 12       | 0.27          |
| (1,324) | 1:27:A:ILE:HD12 | 1:43:A:PHE:HD2  | 12       | 0.27          |
| (1,324) | 1:27:A:ILE:HD13 | 1:43:A:PHE:HD1  | 12       | 0.27          |
| (1,324) | 1:27:A:ILE:HD13 | 1:43:A:PHE:HD2  | 12       | 0.27          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 12       | 0.27          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 6        | 0.27          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 6        | 0.27          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 6        | 0.27          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 19       | 0.27          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 19       | 0.27          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 19       | 0.27          |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 5        | 0.27          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 1        | 0.27          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 1        | 0.27          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 1        | 0.27          |
| (1,249) | 1:15:A:LEU:HD11 | 1:38:A:ALA:H    | 14       | 0.27          |
| (1,249) | 1:15:A:LEU:HD12 | 1:38:A:ALA:H    | 14       | 0.27          |
| (1,249) | 1:15:A:LEU:HD13 | 1:38:A:ALA:H    | 14       | 0.27          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 8        | 0.27          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 8        | 0.27          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 8        | 0.27          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 5        | 0.27          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 11       | 0.27          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD2  | 19       | 0.27          |
| (1,39)  | 1:12:A:LYS:H    | 1:12:A:LYS:HD3  | 19       | 0.27          |
| (2,37)  | 1:48:A:LYS:H    | 1:44:A:HIS:O    | 16       | 0.26          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 3        | 0.26          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 17       | 0.26          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 15       | 0.26          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 19       | 0.26          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 1        | 0.26          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 10       | 0.26          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 20       | 0.26          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 13       | 0.26          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 4        | 0.26          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 19       | 0.26          |
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 3        | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 15       | 0.26          |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 16       | 0.26          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG11 | 17       | 0.26          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG12 | 17       | 0.26          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG13 | 17       | 0.26          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG21 | 17       | 0.26          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG22 | 17       | 0.26          |
| (1,788) | 1:46:A:ARG:H    | 1:49:A:VAL:HG23 | 17       | 0.26          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD11 | 14       | 0.26          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD12 | 14       | 0.26          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD13 | 14       | 0.26          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD21 | 14       | 0.26          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD22 | 14       | 0.26          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD23 | 14       | 0.26          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 4        | 0.26          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 4        | 0.26          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 4        | 0.26          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 4        | 0.26          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 4        | 0.26          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 4        | 0.26          |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 3        | 0.26          |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 3        | 0.26          |
| (1,661) | 1:12:A:LYS:H    | 1:12:A:LYS:HB2  | 16       | 0.26          |
| (1,661) | 1:12:A:LYS:H    | 1:12:A:LYS:HB3  | 16       | 0.26          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 9        | 0.26          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 9        | 0.26          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 9        | 0.26          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 13       | 0.26          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 13       | 0.26          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 13       | 0.26          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 7        | 0.26          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 7        | 0.26          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 7        | 0.26          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 13       | 0.26          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 13       | 0.26          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 13       | 0.26          |
| (1,534) | 1:44:A:HIS:HA   | 1:44:A:HIS:HD2  | 5        | 0.26          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD21 | 10       | 0.26          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD22 | 10       | 0.26          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD23 | 10       | 0.26          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 14       | 0.26          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 17       | 0.26          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 17       | 0.26          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 17       | 0.26          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 14       | 0.26          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 14       | 0.26          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 14       | 0.26          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 19       | 0.26          |
| (1,182) | 1:25:A:ASP:HA   | 1:28:A:ASN:HD21 | 10       | 0.26          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 17       | 0.26          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 17       | 0.26          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 17       | 0.26          |
| (1,165) | 1:3:A:LEU:H     | 1:4:A:GLY:H     | 2        | 0.26          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 10       | 0.26          |
| (1,110) | 1:49:A:VAL:H    | 1:49:A:VAL:HB   | 12       | 0.26          |
| (1,110) | 1:49:A:VAL:H    | 1:49:A:VAL:HB   | 16       | 0.26          |
| (1,37)  | 1:11:A:LYS:HA   | 1:12:A:LYS:H    | 19       | 0.26          |
| (1,26)  | 1:10:A:THR:HA   | 1:11:A:LYS:H    | 15       | 0.26          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB1  | 14       | 0.26          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB2  | 14       | 0.26          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB3  | 14       | 0.26          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 10       | 0.25          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 2        | 0.25          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 4        | 0.25          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 8        | 0.25          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 8        | 0.25          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 19       | 0.25          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 2        | 0.25          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 6        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 9        | 0.25          |
| (2,4)   | 1:24:A:ARG:N    | 1:20:A:TYR:O    | 17       | 0.25          |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 18       | 0.25          |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 3        | 0.25          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD11 | 10       | 0.25          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD12 | 10       | 0.25          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD13 | 10       | 0.25          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD21 | 10       | 0.25          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD22 | 10       | 0.25          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD23 | 10       | 0.25          |
| (1,776) | 1:45:A:ARG:H    | 1:45:A:ARG:HG2  | 19       | 0.25          |
| (1,776) | 1:45:A:ARG:H    | 1:45:A:ARG:HG3  | 19       | 0.25          |
| (1,776) | 1:45:A:ARG:H    | 1:45:A:ARG:HG2  | 20       | 0.25          |
| (1,776) | 1:45:A:ARG:H    | 1:45:A:ARG:HG3  | 20       | 0.25          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 10       | 0.25          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 10       | 0.25          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 10       | 0.25          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 10       | 0.25          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 10       | 0.25          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 10       | 0.25          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 15       | 0.25          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 15       | 0.25          |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 15       | 0.25          |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 15       | 0.25          |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 20       | 0.25          |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 20       | 0.25          |
| (1,644) | 1:48:A:LYS:HD2  | 1:49:A:VAL:H    | 13       | 0.25          |
| (1,644) | 1:48:A:LYS:HD3  | 1:49:A:VAL:H    | 13       | 0.25          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE1  | 18       | 0.25          |
| (1,637) | 1:24:A:ARG:HG3  | 1:43:A:PHE:HE2  | 18       | 0.25          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 19       | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 19       | 0.25          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 19       | 0.25          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 2        | 0.25          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 5        | 0.25          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 5        | 0.25          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 5        | 0.25          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 5        | 0.25          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 15       | 0.25          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 15       | 0.25          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 15       | 0.25          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 3        | 0.25          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 3        | 0.25          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 3        | 0.25          |
| (1,453) | 1:10:A:THR:HG21 | 1:11:A:LYS:H    | 5        | 0.25          |
| (1,453) | 1:10:A:THR:HG22 | 1:11:A:LYS:H    | 5        | 0.25          |
| (1,453) | 1:10:A:THR:HG23 | 1:11:A:LYS:H    | 5        | 0.25          |
| (1,314) | 1:13:A:TYR:H    | 1:15:A:LEU:HD21 | 14       | 0.25          |
| (1,314) | 1:13:A:TYR:H    | 1:15:A:LEU:HD22 | 14       | 0.25          |
| (1,314) | 1:13:A:TYR:H    | 1:15:A:LEU:HD23 | 14       | 0.25          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 18       | 0.25          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 18       | 0.25          |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 11       | 0.25          |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 20       | 0.25          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 7        | 0.25          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 7        | 0.25          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 7        | 0.25          |
| (1,273) | 1:27:A:ILE:HD11 | 1:43:A:PHE:H    | 12       | 0.25          |
| (1,273) | 1:27:A:ILE:HD12 | 1:43:A:PHE:H    | 12       | 0.25          |
| (1,273) | 1:27:A:ILE:HD13 | 1:43:A:PHE:H    | 12       | 0.25          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 4        | 0.25          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 4        | 0.25          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 4        | 0.25          |
| (1,199) | 1:19:A:LYS:HA   | 1:21:A:ALA:H    | 14       | 0.25          |
| (1,199) | 1:19:A:LYS:HA   | 1:21:A:ALA:H    | 20       | 0.25          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 1        | 0.25          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 1        | 0.25          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 1        | 0.25          |
| (1,42)  | 1:3:A:LEU:H     | 1:3:A:LEU:HG    | 6        | 0.25          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 8        | 0.24          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 15       | 0.24          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 6        | 0.24          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 18       | 0.24          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 15       | 0.24          |
| (2,12)  | 1:28:A:ASN:N    | 1:24:A:ARG:O    | 16       | 0.24          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 14       | 0.24          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 3        | 0.24          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 3        | 0.24          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 3        | 0.24          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 3        | 0.24          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 3        | 0.24          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 3        | 0.24          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 7        | 0.24          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 7        | 0.24          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 7        | 0.24          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 7        | 0.24          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 7        | 0.24          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 7        | 0.24          |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE1  | 16       | 0.24          |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE2  | 16       | 0.24          |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE1  | 16       | 0.24          |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE2  | 16       | 0.24          |
| (1,644) | 1:48:A:LYS:HD2  | 1:49:A:VAL:H    | 17       | 0.24          |
| (1,644) | 1:48:A:LYS:HD3  | 1:49:A:VAL:H    | 17       | 0.24          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 11       | 0.24          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 11       | 0.24          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 11       | 0.24          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 1        | 0.24          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 20       | 0.24          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 10       | 0.24          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 10       | 0.24          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 10       | 0.24          |
| (1,453) | 1:10:A:THR:HG21 | 1:11:A:LYS:H    | 16       | 0.24          |
| (1,453) | 1:10:A:THR:HG22 | 1:11:A:LYS:H    | 16       | 0.24          |
| (1,453) | 1:10:A:THR:HG23 | 1:11:A:LYS:H    | 16       | 0.24          |
| (1,431) | 1:21:A:ALA:HA   | 1:24:A:ARG:HB2  | 2        | 0.24          |
| (1,393) | 1:47:A:LEU:H    | 1:47:A:LEU:HG   | 18       | 0.24          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 3        | 0.24          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 3        | 0.24          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 3        | 0.24          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 4        | 0.24          |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 4        | 0.24          |
| (1,251) | 1:36:A:LEU:HD21 | 1:38:A:ALA:H    | 20       | 0.24          |
| (1,251) | 1:36:A:LEU:HD22 | 1:38:A:ALA:H    | 20       | 0.24          |
| (1,251) | 1:36:A:LEU:HD23 | 1:38:A:ALA:H    | 20       | 0.24          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 5        | 0.24          |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 10       | 0.24          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 20       | 0.24          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 1        | 0.24          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 11       | 0.24          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 13       | 0.24          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 17       | 0.24          |
| (1,91)  | 1:34:A:GLU:HA   | 1:37:A:ALA:H    | 3        | 0.24          |
| (1,42)  | 1:3:A:LEU:H     | 1:3:A:LEU:HG    | 3        | 0.24          |
| (1,36)  | 1:11:A:LYS:H    | 1:12:A:LYS:H    | 1        | 0.24          |
| (1,23)  | 1:30:A:SER:HG   | 1:32:A:ASP:H    | 13       | 0.24          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB1  | 19       | 0.24          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB2  | 19       | 0.24          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB3  | 19       | 0.24          |
| (2,38)  | 1:48:A:LYS:N    | 1:44:A:HIS:O    | 9        | 0.23          |
| (2,37)  | 1:48:A:LYS:H    | 1:44:A:HIS:O    | 1        | 0.23          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 20       | 0.23          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 12       | 0.23          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 3        | 0.23          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 16       | 0.23          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 18       | 0.23          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 14       | 0.23          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 13       | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 6        | 0.23          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 7        | 0.23          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 9        | 0.23          |
| (2,19)  | 1:38:A:ALA:H    | 1:34:A:GLU:O    | 3        | 0.23          |
| (2,5)   | 1:25:A:ASP:H    | 1:21:A:ALA:O    | 9        | 0.23          |
| (2,4)   | 1:24:A:ARG:N    | 1:20:A:TYR:O    | 16       | 0.23          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 18       | 0.23          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 18       | 0.23          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 18       | 0.23          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 18       | 0.23          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 18       | 0.23          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 18       | 0.23          |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 14       | 0.23          |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 14       | 0.23          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 9        | 0.23          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 9        | 0.23          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 9        | 0.23          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 10       | 0.23          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 10       | 0.23          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 10       | 0.23          |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 4        | 0.23          |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 4        | 0.23          |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 4        | 0.23          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 4        | 0.23          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 4        | 0.23          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 4        | 0.23          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 15       | 0.23          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 15       | 0.23          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 15       | 0.23          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD21 | 18       | 0.23          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD22 | 18       | 0.23          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD23 | 18       | 0.23          |
| (1,431) | 1:21:A:ALA:HA   | 1:24:A:ARG:HB2  | 13       | 0.23          |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB1  | 4        | 0.23          |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB2  | 4        | 0.23          |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB3  | 4        | 0.23          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 5        | 0.23          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 5        | 0.23          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 5        | 0.23          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 6        | 0.23          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 6        | 0.23          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 6        | 0.23          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 8        | 0.23          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 9        | 0.23          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 10       | 0.23          |
| (1,291) | 1:38:A:ALA:H    | 1:41:A:GLU:HB2  | 5        | 0.23          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 14       | 0.23          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 14       | 0.23          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 14       | 0.23          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 20       | 0.23          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 20       | 0.23          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 20       | 0.23          |
| (1,273) | 1:27:A:ILE:HD11 | 1:43:A:PHE:H    | 8        | 0.23          |
| (1,273) | 1:27:A:ILE:HD12 | 1:43:A:PHE:H    | 8        | 0.23          |
| (1,273) | 1:27:A:ILE:HD13 | 1:43:A:PHE:H    | 8        | 0.23          |
| (1,199) | 1:19:A:LYS:HA   | 1:21:A:ALA:H    | 9        | 0.23          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 5        | 0.23          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 10       | 0.23          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 16       | 0.23          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 19       | 0.23          |
| (1,183) | 1:27:A:ILE:H    | 1:28:A:ASN:HB2  | 7        | 0.23          |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD2  | 19       | 0.23          |
| (1,130) | 1:17:A:LYS:H    | 1:17:A:LYS:HD3  | 19       | 0.23          |
| (1,36)  | 1:11:A:LYS:H    | 1:12:A:LYS:H    | 14       | 0.23          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB1  | 9        | 0.23          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB2  | 9        | 0.23          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB3  | 9        | 0.23          |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 4        | 0.23          |
| (2,38)  | 1:48:A:LYS:N    | 1:44:A:HIS:O    | 16       | 0.22          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 16       | 0.22          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 15       | 0.22          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 2        | 0.22          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 15       | 0.22          |
| (2,4)   | 1:24:A:ARG:N    | 1:20:A:TYR:O    | 18       | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 8        | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 8        | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 8        | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 8        | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 8        | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 8        | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 11       | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 11       | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 11       | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 11       | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 11       | 0.22          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 11       | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD11 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD12 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD13 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD21 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD22 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD23 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD11 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD12 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD13 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD21 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD22 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD23 | 5        | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD11 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD12 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD13 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD21 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD22 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD23 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD11 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD12 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD13 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD21 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD22 | 19       | 0.22          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD23 | 19       | 0.22          |
| (1,718) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HG2  | 2        | 0.22          |
| (1,718) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HG3  | 2        | 0.22          |
| (1,718) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HG2  | 2        | 0.22          |
| (1,718) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HG3  | 2        | 0.22          |
| (1,718) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HG2  | 2        | 0.22          |
| (1,718) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HG3  | 2        | 0.22          |
| (1,664) | 1:12:A:LYS:HB2  | 1:13:A:TYR:H    | 7        | 0.22          |
| (1,664) | 1:12:A:LYS:HB3  | 1:13:A:TYR:H    | 7        | 0.22          |
| (1,662) | 1:12:A:LYS:H    | 1:12:A:LYS:HG2  | 4        | 0.22          |
| (1,662) | 1:12:A:LYS:H    | 1:12:A:LYS:HG3  | 4        | 0.22          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 12       | 0.22          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 12       | 0.22          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 12       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 7        | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 7        | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 7        | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 7        | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 7        | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 7        | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 7        | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 7        | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 7        | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 8        | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 13       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 14       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 15       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 15       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 15       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 15       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 15       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 15       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 15       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 15       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 15       | 0.22          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 20       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 20       | 0.22          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 20       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 20       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 20       | 0.22          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 20       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 20       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 20       | 0.22          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 20       | 0.22          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 15       | 0.22          |
| (1,586) | 1:44:A:HIS:HA   | 1:47:A:LEU:HG   | 2        | 0.22          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 13       | 0.22          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 13       | 0.22          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 13       | 0.22          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 16       | 0.22          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 16       | 0.22          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 16       | 0.22          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 1        | 0.22          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 1        | 0.22          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 1        | 0.22          |
| (1,509) | 1:19:A:LYS:HA   | 1:19:A:LYS:HD2  | 9        | 0.22          |
| (1,491) | 1:27:A:ILE:HA   | 1:32:A:ASP:H    | 8        | 0.22          |
| (1,361) | 1:49:A:VAL:HA   | 1:50:A:TYR:H    | 10       | 0.22          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 20       | 0.22          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 20       | 0.22          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 4        | 0.22          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 4        | 0.22          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 4        | 0.22          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 20       | 0.22          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 20       | 0.22          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 20       | 0.22          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 5        | 0.22          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 5        | 0.22          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 9        | 0.22          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 9        | 0.22          |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 19       | 0.22          |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 8        | 0.22          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 5        | 0.22          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 5        | 0.22          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 5        | 0.22          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 4        | 0.22          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 7        | 0.22          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,189) | 1:18:A:TRP:HZ3 | 1:26:A:THR:H    | 9        | 0.22          |
| (1,130) | 1:17:A:LYS:H   | 1:17:A:LYS:HD2  | 9        | 0.22          |
| (1,130) | 1:17:A:LYS:H   | 1:17:A:LYS:HD3  | 9        | 0.22          |
| (1,28)  | 1:11:A:LYS:H   | 1:11:A:LYS:HG2  | 14       | 0.22          |
| (1,10)  | 1:50:A:TYR:H   | 1:51:A:HIS:H    | 18       | 0.22          |
| (2,32)  | 1:44:A:HIS:N   | 1:40:A:ARG:O    | 8        | 0.21          |
| (2,32)  | 1:44:A:HIS:N   | 1:40:A:ARG:O    | 14       | 0.21          |
| (2,9)   | 1:27:A:ILE:H   | 1:23:A:LEU:O    | 8        | 0.21          |
| (2,5)   | 1:25:A:ASP:H   | 1:21:A:ALA:O    | 16       | 0.21          |
| (2,1)   | 1:23:A:LEU:H   | 1:19:A:LYS:O    | 4        | 0.21          |
| (2,1)   | 1:23:A:LEU:H   | 1:19:A:LYS:O    | 17       | 0.21          |
| (1,770) | 1:44:A:HIS:H   | 1:47:A:LEU:HD11 | 5        | 0.21          |
| (1,770) | 1:44:A:HIS:H   | 1:47:A:LEU:HD12 | 5        | 0.21          |
| (1,770) | 1:44:A:HIS:H   | 1:47:A:LEU:HD13 | 5        | 0.21          |
| (1,770) | 1:44:A:HIS:H   | 1:47:A:LEU:HD21 | 5        | 0.21          |
| (1,770) | 1:44:A:HIS:H   | 1:47:A:LEU:HD22 | 5        | 0.21          |
| (1,770) | 1:44:A:HIS:H   | 1:47:A:LEU:HD23 | 5        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD13 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD21 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD22 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD23 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD11 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD12 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD13 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD21 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD22 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD23 | 3        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD13 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD21 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD22 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD23 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD11 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD12 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD13 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD21 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD22 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD23 | 4        | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 12       | 0.21          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD13 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD21 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD22 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD23 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD11 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD12 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD13 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD21 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD22 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD23 | 12       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD13 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD21 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD22 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD23 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD11 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD12 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD13 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD21 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD22 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD23 | 15       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD13 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD21 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD22 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD23 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD11 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD12 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD13 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD21 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD22 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD23 | 18       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD13 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD21 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD22 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD23 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD11 | 20       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD12 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD13 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD21 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD22 | 20       | 0.21          |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD23 | 20       | 0.21          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 12       | 0.21          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 12       | 0.21          |
| (1,710) | 1:24:A:ARG:HD2  | 1:25:A:ASP:H    | 5        | 0.21          |
| (1,710) | 1:24:A:ARG:HD3  | 1:25:A:ASP:H    | 5        | 0.21          |
| (1,685) | 1:19:A:LYS:H    | 1:19:A:LYS:HD2  | 16       | 0.21          |
| (1,685) | 1:19:A:LYS:H    | 1:19:A:LYS:HD3  | 16       | 0.21          |
| (1,679) | 1:17:A:LYS:H    | 1:17:A:LYS:HG2  | 12       | 0.21          |
| (1,679) | 1:17:A:LYS:H    | 1:17:A:LYS:HG3  | 12       | 0.21          |
| (1,679) | 1:17:A:LYS:H    | 1:17:A:LYS:HG2  | 15       | 0.21          |
| (1,679) | 1:17:A:LYS:H    | 1:17:A:LYS:HG3  | 15       | 0.21          |
| (1,664) | 1:12:A:LYS:HB2  | 1:13:A:TYR:H    | 3        | 0.21          |
| (1,664) | 1:12:A:LYS:HB3  | 1:13:A:TYR:H    | 3        | 0.21          |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE1  | 12       | 0.21          |
| (1,653) | 1:12:A:LYS:HD2  | 1:13:A:TYR:HE2  | 12       | 0.21          |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE1  | 12       | 0.21          |
| (1,653) | 1:12:A:LYS:HD3  | 1:13:A:TYR:HE2  | 12       | 0.21          |
| (1,624) | 1:15:A:LEU:HD11 | 1:39:A:CYS:HA   | 12       | 0.21          |
| (1,624) | 1:15:A:LEU:HD12 | 1:39:A:CYS:HA   | 12       | 0.21          |
| (1,624) | 1:15:A:LEU:HD13 | 1:39:A:CYS:HA   | 12       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 1        | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 2        | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 2        | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 2        | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 2        | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 2        | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 2        | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 2        | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 2        | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 2        | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 10       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 11       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 16       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 18       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 18       | 0.21          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 18       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 18       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 18       | 0.21          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 18       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 18       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 18       | 0.21          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 18       | 0.21          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 10       | 0.21          |
| (1,534) | 1:44:A:HIS:HA   | 1:44:A:HIS:HD2  | 7        | 0.21          |
| (1,491) | 1:27:A:ILE:HA   | 1:32:A:ASP:H    | 7        | 0.21          |
| (1,491) | 1:27:A:ILE:HA   | 1:32:A:ASP:H    | 14       | 0.21          |
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD21 | 10       | 0.21          |
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD22 | 10       | 0.21          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,435) | 1:43:A:PHE:HD1  | 1:47:A:LEU:HD23 | 10       | 0.21          |
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD21 | 10       | 0.21          |
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD22 | 10       | 0.21          |
| (1,435) | 1:43:A:PHE:HD2  | 1:47:A:LEU:HD23 | 10       | 0.21          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD21 | 9        | 0.21          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD22 | 9        | 0.21          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD23 | 9        | 0.21          |
| (1,414) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HA   | 8        | 0.21          |
| (1,414) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HA   | 8        | 0.21          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 13       | 0.21          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 13       | 0.21          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD11 | 3        | 0.21          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD12 | 3        | 0.21          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD13 | 3        | 0.21          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 12       | 0.21          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 12       | 0.21          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 12       | 0.21          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 14       | 0.21          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 14       | 0.21          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 14       | 0.21          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 1        | 0.21          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 10       | 0.21          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 10       | 0.21          |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 8        | 0.21          |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 6        | 0.21          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 7        | 0.21          |
| (1,273) | 1:27:A:ILE:HD11 | 1:43:A:PHE:H    | 6        | 0.21          |
| (1,273) | 1:27:A:ILE:HD12 | 1:43:A:PHE:H    | 6        | 0.21          |
| (1,273) | 1:27:A:ILE:HD13 | 1:43:A:PHE:H    | 6        | 0.21          |
| (1,268) | 1:38:A:ALA:H    | 1:41:A:GLU:H    | 5        | 0.21          |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 6        | 0.21          |
| (1,260) | 1:27:A:ILE:HG21 | 1:40:A:ARG:H    | 2        | 0.21          |
| (1,260) | 1:27:A:ILE:HG22 | 1:40:A:ARG:H    | 2        | 0.21          |
| (1,260) | 1:27:A:ILE:HG23 | 1:40:A:ARG:H    | 2        | 0.21          |
| (1,254) | 1:15:A:LEU:HD11 | 1:39:A:CYS:H    | 3        | 0.21          |
| (1,254) | 1:15:A:LEU:HD12 | 1:39:A:CYS:H    | 3        | 0.21          |
| (1,254) | 1:15:A:LEU:HD13 | 1:39:A:CYS:H    | 3        | 0.21          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 4        | 0.21          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 14       | 0.21          |
| (1,185) | 1:26:A:THR:HG1  | 1:27:A:ILE:H    | 15       | 0.21          |
| (1,182) | 1:25:A:ASP:HA   | 1:28:A:ASN:HD21 | 14       | 0.21          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 9        | 0.21          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,42)  | 1:3:A:LEU:H    | 1:3:A:LEU:HG    | 17       | 0.21          |
| (1,36)  | 1:11:A:LYS:H   | 1:12:A:LYS:H    | 12       | 0.21          |
| (1,10)  | 1:50:A:TYR:H   | 1:51:A:HIS:H    | 14       | 0.21          |
| (2,37)  | 1:48:A:LYS:H   | 1:44:A:HIS:O    | 8        | 0.2           |
| (2,34)  | 1:45:A:ARG:N   | 1:41:A:GLU:O    | 12       | 0.2           |
| (2,33)  | 1:45:A:ARG:H   | 1:41:A:GLU:O    | 19       | 0.2           |
| (2,32)  | 1:44:A:HIS:N   | 1:40:A:ARG:O    | 3        | 0.2           |
| (2,32)  | 1:44:A:HIS:N   | 1:40:A:ARG:O    | 13       | 0.2           |
| (2,32)  | 1:44:A:HIS:N   | 1:40:A:ARG:O    | 16       | 0.2           |
| (2,28)  | 1:42:A:GLU:N   | 1:38:A:ALA:O    | 6        | 0.2           |
| (2,27)  | 1:42:A:GLU:H   | 1:38:A:ALA:O    | 11       | 0.2           |
| (2,23)  | 1:40:A:ARG:H   | 1:36:A:LEU:O    | 10       | 0.2           |
| (2,13)  | 1:29:A:THR:H   | 1:25:A:ASP:O    | 7        | 0.2           |
| (2,12)  | 1:28:A:ASN:N   | 1:24:A:ARG:O    | 17       | 0.2           |
| (2,11)  | 1:28:A:ASN:H   | 1:24:A:ARG:O    | 3        | 0.2           |
| (2,11)  | 1:28:A:ASN:H   | 1:24:A:ARG:O    | 7        | 0.2           |
| (2,11)  | 1:28:A:ASN:H   | 1:24:A:ARG:O    | 12       | 0.2           |
| (2,11)  | 1:28:A:ASN:H   | 1:24:A:ARG:O    | 14       | 0.2           |
| (2,1)   | 1:23:A:LEU:H   | 1:19:A:LYS:O    | 2        | 0.2           |
| (2,1)   | 1:23:A:LEU:H   | 1:19:A:LYS:O    | 18       | 0.2           |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD11 | 20       | 0.2           |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD12 | 20       | 0.2           |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD13 | 20       | 0.2           |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD21 | 20       | 0.2           |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD22 | 20       | 0.2           |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD23 | 20       | 0.2           |
| (1,776) | 1:45:A:ARG:H   | 1:45:A:ARG:HG2  | 2        | 0.2           |
| (1,776) | 1:45:A:ARG:H   | 1:45:A:ARG:HG3  | 2        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD13 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD21 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD22 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD23 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD11 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD12 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD13 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD21 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD22 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD23 | 7        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 8        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD13 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD21 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD22 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD23 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD11 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD12 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD13 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD21 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD22 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD23 | 8        | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD11 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD12 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD13 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD21 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD22 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD23 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD11 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD12 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD13 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD21 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD22 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD23 | 10       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD11 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD12 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD13 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD21 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD22 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB2  | 1:47:A:LEU:HD23 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD11 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD12 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD13 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD21 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD22 | 17       | 0.2           |
| (1,765) | 1:43:A:PHE:HB3  | 1:47:A:LEU:HD23 | 17       | 0.2           |
| (1,640) | 1:19:A:LYS:HA   | 1:19:A:LYS:HD3  | 1        | 0.2           |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 4        | 0.2           |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 4        | 0.2           |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 4        | 0.2           |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 3        | 0.2           |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 3        | 0.2           |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 3        | 0.2           |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 3        | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 3        | 0.2           |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 3        | 0.2           |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 3        | 0.2           |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 3        | 0.2           |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 3        | 0.2           |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 3        | 0.2           |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 3        | 0.2           |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 3        | 0.2           |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD11 | 19       | 0.2           |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD12 | 19       | 0.2           |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD13 | 19       | 0.2           |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD11 | 19       | 0.2           |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD12 | 19       | 0.2           |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD13 | 19       | 0.2           |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD11 | 19       | 0.2           |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD12 | 19       | 0.2           |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD13 | 19       | 0.2           |
| (1,534) | 1:44:A:HIS:HA   | 1:44:A:HIS:HD2  | 8        | 0.2           |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 18       | 0.2           |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 18       | 0.2           |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 18       | 0.2           |
| (1,491) | 1:27:A:ILE:HA   | 1:32:A:ASP:H    | 4        | 0.2           |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB1  | 6        | 0.2           |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB2  | 6        | 0.2           |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB3  | 6        | 0.2           |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB1  | 6        | 0.2           |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB2  | 6        | 0.2           |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB3  | 6        | 0.2           |
| (1,464) | 1:15:A:LEU:HD21 | 1:18:A:TRP:HZ3  | 19       | 0.2           |
| (1,464) | 1:15:A:LEU:HD22 | 1:18:A:TRP:HZ3  | 19       | 0.2           |
| (1,464) | 1:15:A:LEU:HD23 | 1:18:A:TRP:HZ3  | 19       | 0.2           |
| (1,451) | 1:15:A:LEU:HD11 | 1:35:A:LEU:HD21 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD11 | 1:35:A:LEU:HD22 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD11 | 1:35:A:LEU:HD23 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD12 | 1:35:A:LEU:HD21 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD12 | 1:35:A:LEU:HD22 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD12 | 1:35:A:LEU:HD23 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD13 | 1:35:A:LEU:HD21 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD13 | 1:35:A:LEU:HD22 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD13 | 1:35:A:LEU:HD23 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD21 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD22 | 12       | 0.2           |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,451) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD23 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD21 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD22 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD23 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD21 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD22 | 12       | 0.2           |
| (1,451) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD23 | 12       | 0.2           |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 9        | 0.2           |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 9        | 0.2           |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 9        | 0.2           |
| (1,361) | 1:49:A:VAL:HA   | 1:50:A:TYR:H    | 1        | 0.2           |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB1  | 1        | 0.2           |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB2  | 1        | 0.2           |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB3  | 1        | 0.2           |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 13       | 0.2           |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 13       | 0.2           |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 13       | 0.2           |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 15       | 0.2           |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 15       | 0.2           |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 9        | 0.2           |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 16       | 0.2           |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 17       | 0.2           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 9        | 0.2           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 9        | 0.2           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 9        | 0.2           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 11       | 0.2           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 11       | 0.2           |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 11       | 0.2           |
| (1,277) | 1:44:A:HIS:H    | 1:44:A:HIS:HD2  | 7        | 0.2           |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 17       | 0.2           |
| (1,226) | 1:26:A:THR:HG21 | 1:31:A:CYS:H    | 3        | 0.2           |
| (1,226) | 1:26:A:THR:HG22 | 1:31:A:CYS:H    | 3        | 0.2           |
| (1,226) | 1:26:A:THR:HG23 | 1:31:A:CYS:H    | 3        | 0.2           |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 5        | 0.2           |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 15       | 0.2           |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 12       | 0.2           |
| (1,35)  | 1:19:A:LYS:H    | 1:19:A:LYS:HG2  | 16       | 0.2           |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 12       | 0.19          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 8        | 0.19          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 5        | 0.19          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 3        | 0.19          |
| (1,796) | 1:47:A:LEU:HA   | 1:47:A:LEU:HD11 | 18       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,796) | 1:47:A:LEU:HA   | 1:47:A:LEU:HD12 | 18       | 0.19          |
| (1,796) | 1:47:A:LEU:HA   | 1:47:A:LEU:HD13 | 18       | 0.19          |
| (1,796) | 1:47:A:LEU:HA   | 1:47:A:LEU:HD21 | 18       | 0.19          |
| (1,796) | 1:47:A:LEU:HA   | 1:47:A:LEU:HD22 | 18       | 0.19          |
| (1,796) | 1:47:A:LEU:HA   | 1:47:A:LEU:HD23 | 18       | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD11 | 4        | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD12 | 4        | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD13 | 4        | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD21 | 4        | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD22 | 4        | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD23 | 4        | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD11 | 19       | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD12 | 19       | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD13 | 19       | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD21 | 19       | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD22 | 19       | 0.19          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD23 | 19       | 0.19          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 13       | 0.19          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 13       | 0.19          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 13       | 0.19          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 13       | 0.19          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 13       | 0.19          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 13       | 0.19          |
| (1,644) | 1:48:A:LYS:HD2  | 1:49:A:VAL:H    | 2        | 0.19          |
| (1,644) | 1:48:A:LYS:HD3  | 1:49:A:VAL:H    | 2        | 0.19          |
| (1,643) | 1:48:A:LYS:H    | 1:48:A:LYS:HD2  | 4        | 0.19          |
| (1,643) | 1:48:A:LYS:H    | 1:48:A:LYS:HD3  | 4        | 0.19          |
| (1,634) | 1:29:A:THR:H    | 1:30:A:SER:HB3  | 16       | 0.19          |
| (1,624) | 1:15:A:LEU:HD11 | 1:39:A:CYS:HA   | 3        | 0.19          |
| (1,624) | 1:15:A:LEU:HD12 | 1:39:A:CYS:HA   | 3        | 0.19          |
| (1,624) | 1:15:A:LEU:HD13 | 1:39:A:CYS:HA   | 3        | 0.19          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 4        | 0.19          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 9        | 0.19          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 9        | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 9        | 0.19          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 9        | 0.19          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 9        | 0.19          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 9        | 0.19          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 9        | 0.19          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 9        | 0.19          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 9        | 0.19          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 11       | 0.19          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 11       | 0.19          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 11       | 0.19          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 16       | 0.19          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 16       | 0.19          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 16       | 0.19          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 17       | 0.19          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 17       | 0.19          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 17       | 0.19          |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB1  | 4        | 0.19          |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB2  | 4        | 0.19          |
| (1,477) | 1:13:A:TYR:HE1  | 1:38:A:ALA:HB3  | 4        | 0.19          |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB1  | 4        | 0.19          |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB2  | 4        | 0.19          |
| (1,477) | 1:13:A:TYR:HE2  | 1:38:A:ALA:HB3  | 4        | 0.19          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 16       | 0.19          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 16       | 0.19          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 16       | 0.19          |
| (1,432) | 1:21:A:ALA:HA   | 1:24:A:ARG:HG2  | 16       | 0.19          |
| (1,431) | 1:21:A:ALA:HA   | 1:24:A:ARG:HB2  | 18       | 0.19          |
| (1,414) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HA   | 10       | 0.19          |
| (1,414) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HA   | 10       | 0.19          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 7        | 0.19          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 7        | 0.19          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 7        | 0.19          |
| (1,324) | 1:27:A:ILE:HD11 | 1:43:A:PHE:HD1  | 5        | 0.19          |
| (1,324) | 1:27:A:ILE:HD11 | 1:43:A:PHE:HD2  | 5        | 0.19          |
| (1,324) | 1:27:A:ILE:HD12 | 1:43:A:PHE:HD1  | 5        | 0.19          |
| (1,324) | 1:27:A:ILE:HD12 | 1:43:A:PHE:HD2  | 5        | 0.19          |
| (1,324) | 1:27:A:ILE:HD13 | 1:43:A:PHE:HD1  | 5        | 0.19          |
| (1,324) | 1:27:A:ILE:HD13 | 1:43:A:PHE:HD2  | 5        | 0.19          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 11       | 0.19          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 11       | 0.19          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 11       | 0.19          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 20       | 0.19          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 20       | 0.19          |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 10       | 0.19          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 17       | 0.19          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 17       | 0.19          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 17       | 0.19          |
| (1,277) | 1:44:A:HIS:H    | 1:44:A:HIS:HD2  | 5        | 0.19          |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 7        | 0.19          |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 13       | 0.19          |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 15       | 0.19          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 14       | 0.19          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 8        | 0.19          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD21 | 15       | 0.19          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD22 | 15       | 0.19          |
| (1,172) | 1:29:A:THR:H    | 1:36:A:LEU:HD23 | 15       | 0.19          |
| (1,36)  | 1:11:A:LYS:H    | 1:12:A:LYS:H    | 3        | 0.19          |
| (1,36)  | 1:11:A:LYS:H    | 1:12:A:LYS:H    | 15       | 0.19          |
| (1,13)  | 1:50:A:TYR:HA   | 1:51:A:HIS:H    | 9        | 0.19          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 15       | 0.18          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 16       | 0.18          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 6        | 0.18          |
| (2,24)  | 1:40:A:ARG:N    | 1:36:A:LEU:O    | 8        | 0.18          |
| (2,20)  | 1:38:A:ALA:N    | 1:34:A:GLU:O    | 3        | 0.18          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 12       | 0.18          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 19       | 0.18          |
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 6        | 0.18          |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 6        | 0.18          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 6        | 0.18          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 7        | 0.18          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 20       | 0.18          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 15       | 0.18          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 15       | 0.18          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 15       | 0.18          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 15       | 0.18          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 15       | 0.18          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 15       | 0.18          |
| (1,754) | 1:41:A:GLU:HA   | 1:44:A:HIS:HB2  | 15       | 0.18          |
| (1,754) | 1:41:A:GLU:HA   | 1:44:A:HIS:HB3  | 15       | 0.18          |
| (1,751) | 1:41:A:GLU:H    | 1:41:A:GLU:HG2  | 10       | 0.18          |
| (1,751) | 1:41:A:GLU:H    | 1:41:A:GLU:HG3  | 10       | 0.18          |
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 12       | 0.18          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 7        | 0.18          |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 13       | 0.18          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 13       | 0.18          |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 13       | 0.18          |
| (1,519) | 1:32:A:ASP:HB2  | 1:35:A:LEU:HG   | 9        | 0.18          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 1        | 0.18          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 1        | 0.18          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 1        | 0.18          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD21 | 12       | 0.18          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD22 | 12       | 0.18          |
| (1,449) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HD23 | 12       | 0.18          |
| (1,374) | 1:48:A:LYS:HA   | 1:48:A:LYS:HD2  | 16       | 0.18          |
| (1,374) | 1:48:A:LYS:HA   | 1:48:A:LYS:HD3  | 16       | 0.18          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 19       | 0.18          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 20       | 0.18          |
| (1,301) | 1:17:A:LYS:H    | 1:18:A:TRP:HB2  | 13       | 0.18          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 4        | 0.18          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 4        | 0.18          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 8        | 0.18          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 8        | 0.18          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 19       | 0.18          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 19       | 0.18          |
| (1,282) | 1:43:A:PHE:HA   | 1:46:A:ARG:HE   | 5        | 0.18          |
| (1,273) | 1:27:A:ILE:HD11 | 1:43:A:PHE:H    | 4        | 0.18          |
| (1,273) | 1:27:A:ILE:HD12 | 1:43:A:PHE:H    | 4        | 0.18          |
| (1,273) | 1:27:A:ILE:HD13 | 1:43:A:PHE:H    | 4        | 0.18          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 1        | 0.18          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 1        | 0.18          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 1        | 0.18          |
| (1,205) | 1:19:A:LYS:H    | 1:23:A:LEU:HB2  | 13       | 0.18          |
| (1,184) | 1:23:A:LEU:HA   | 1:27:A:ILE:H    | 12       | 0.18          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 15       | 0.18          |
| (1,120) | 1:26:A:THR:H    | 1:26:A:THR:HG1  | 20       | 0.18          |
| (1,110) | 1:49:A:VAL:H    | 1:49:A:VAL:HB   | 19       | 0.18          |
| (1,96)  | 1:40:A:ARG:H    | 1:40:A:ARG:HG3  | 2        | 0.18          |
| (1,88)  | 1:41:A:GLU:HA   | 1:45:A:ARG:H    | 18       | 0.18          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB2  | 15       | 0.18          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 15       | 0.18          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 5        | 0.17          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 3        | 0.17          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 17       | 0.17          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 5        | 0.17          |
| (2,28)  | 1:42:A:GLU:N    | 1:38:A:ALA:O    | 11       | 0.17          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 3        | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 13       | 0.17          |
| (2,24)  | 1:40:A:ARG:N    | 1:36:A:LEU:O    | 4        | 0.17          |
| (2,10)  | 1:27:A:ILE:N    | 1:23:A:LEU:O    | 12       | 0.17          |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 4        | 0.17          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 15       | 0.17          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG11 | 18       | 0.17          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG12 | 18       | 0.17          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG13 | 18       | 0.17          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG21 | 18       | 0.17          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG22 | 18       | 0.17          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG23 | 18       | 0.17          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD11 | 17       | 0.17          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD12 | 17       | 0.17          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD13 | 17       | 0.17          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD21 | 17       | 0.17          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD22 | 17       | 0.17          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD23 | 17       | 0.17          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD11 | 17       | 0.17          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD12 | 17       | 0.17          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD13 | 17       | 0.17          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD21 | 17       | 0.17          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD22 | 17       | 0.17          |
| (1,770) | 1:44:A:HIS:H    | 1:47:A:LEU:HD23 | 17       | 0.17          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 1        | 0.17          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 1        | 0.17          |
| (1,704) | 1:24:A:ARG:H    | 1:24:A:ARG:HD2  | 5        | 0.17          |
| (1,704) | 1:24:A:ARG:H    | 1:24:A:ARG:HD3  | 5        | 0.17          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 14       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 14       | 0.17          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 14       | 0.17          |
| (1,491) | 1:27:A:ILE:HA   | 1:32:A:ASP:H    | 12       | 0.17          |
| (1,491) | 1:27:A:ILE:HA   | 1:32:A:ASP:H    | 19       | 0.17          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD21 | 17       | 0.17          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD22 | 17       | 0.17          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD23 | 17       | 0.17          |
| (1,392) | 1:18:A:TRP:HZ3  | 1:23:A:LEU:HA   | 16       | 0.17          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 11       | 0.17          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 11       | 0.17          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 11       | 0.17          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 15       | 0.17          |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 13       | 0.17          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 1        | 0.17          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 1        | 0.17          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 1        | 0.17          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 5        | 0.17          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 5        | 0.17          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 5        | 0.17          |
| (1,273) | 1:27:A:ILE:HD11 | 1:43:A:PHE:H    | 10       | 0.17          |
| (1,273) | 1:27:A:ILE:HD12 | 1:43:A:PHE:H    | 10       | 0.17          |
| (1,273) | 1:27:A:ILE:HD13 | 1:43:A:PHE:H    | 10       | 0.17          |
| (1,269) | 1:15:A:LEU:HD11 | 1:42:A:GLU:H    | 2        | 0.17          |
| (1,269) | 1:15:A:LEU:HD12 | 1:42:A:GLU:H    | 2        | 0.17          |
| (1,269) | 1:15:A:LEU:HD13 | 1:42:A:GLU:H    | 2        | 0.17          |
| (1,268) | 1:38:A:ALA:H    | 1:41:A:GLU:H    | 4        | 0.17          |
| (1,268) | 1:38:A:ALA:H    | 1:41:A:GLU:H    | 11       | 0.17          |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 11       | 0.17          |
| (1,261) | 1:27:A:ILE:HG12 | 1:40:A:ARG:H    | 14       | 0.17          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 8        | 0.17          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 8        | 0.17          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 8        | 0.17          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 11       | 0.17          |
| (1,189) | 1:18:A:TRP:HZ3  | 1:26:A:THR:H    | 20       | 0.17          |
| (1,183) | 1:27:A:ILE:H    | 1:28:A:ASN:HB2  | 20       | 0.17          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 1        | 0.17          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 19       | 0.17          |
| (1,150) | 1:14:A:ASP:HA   | 1:16:A:SER:H    | 2        | 0.17          |
| (1,88)  | 1:41:A:GLU:HA   | 1:45:A:ARG:H    | 2        | 0.17          |
| (1,88)  | 1:41:A:GLU:HA   | 1:45:A:ARG:H    | 3        | 0.17          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB2  | 10       | 0.17          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 10       | 0.17          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB1  | 13       | 0.17          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB2  | 13       | 0.17          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB3  | 13       | 0.17          |
| (2,38)  | 1:48:A:LYS:N    | 1:44:A:HIS:O    | 8        | 0.16          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 19       | 0.16          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 7        | 0.16          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 5        | 0.16          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 13       | 0.16          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 15       | 0.16          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 17       | 0.16          |
| (2,6)   | 1:25:A:ASP:N    | 1:21:A:ALA:O    | 19       | 0.16          |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 2        | 0.16          |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 14       | 0.16          |
| (1,754) | 1:41:A:GLU:HA   | 1:44:A:HIS:HB2  | 18       | 0.16          |
| (1,754) | 1:41:A:GLU:HA   | 1:44:A:HIS:HB3  | 18       | 0.16          |
| (1,751) | 1:41:A:GLU:H    | 1:41:A:GLU:HG2  | 6        | 0.16          |
| (1,751) | 1:41:A:GLU:H    | 1:41:A:GLU:HG3  | 6        | 0.16          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 8        | 0.16          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 8        | 0.16          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 2        | 0.16          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 2        | 0.16          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 2        | 0.16          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 12       | 0.16          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD11 | 19       | 0.16          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD12 | 19       | 0.16          |
| (1,601) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD13 | 19       | 0.16          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD11 | 19       | 0.16          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD12 | 19       | 0.16          |
| (1,601) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD13 | 19       | 0.16          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD11 | 19       | 0.16          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD12 | 19       | 0.16          |
| (1,601) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD13 | 19       | 0.16          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 2        | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 2        | 0.16          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 2        | 0.16          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD11 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD12 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD13 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD11 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD12 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD13 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD11 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD12 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD13 | 5        | 0.16          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD11 | 18       | 0.16          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD12 | 18       | 0.16          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD13 | 18       | 0.16          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD11 | 18       | 0.16          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD12 | 18       | 0.16          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD13 | 18       | 0.16          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD11 | 18       | 0.16          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD12 | 18       | 0.16          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD13 | 18       | 0.16          |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 3        | 0.16          |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 3        | 0.16          |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 3        | 0.16          |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 7        | 0.16          |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 7        | 0.16          |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 7        | 0.16          |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 15       | 0.16          |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 15       | 0.16          |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 15       | 0.16          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 3        | 0.16          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 3        | 0.16          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 3        | 0.16          |
| (1,392) | 1:18:A:TRP:HZ3  | 1:23:A:LEU:HA   | 9        | 0.16          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 12       | 0.16          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 12       | 0.16          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 14       | 0.16          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 14       | 0.16          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD11 | 6        | 0.16          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD12 | 6        | 0.16          |
| (1,353) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD13 | 6        | 0.16          |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 3        | 0.16          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD21 | 10       | 0.16          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD22 | 10       | 0.16          |
| (1,286) | 1:28:A:ASN:H    | 1:36:A:LEU:HD23 | 10       | 0.16          |
| (1,277) | 1:44:A:HIS:H    | 1:44:A:HIS:HD2  | 3        | 0.16          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 16       | 0.16          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 19       | 0.16          |
| (1,202) | 1:19:A:LYS:H    | 1:21:A:ALA:H    | 7        | 0.16          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 3        | 0.16          |
| (1,182) | 1:25:A:ASP:HA   | 1:28:A:ASN:HD21 | 1        | 0.16          |
| (1,168) | 1:27:A:ILE:HA   | 1:29:A:THR:H    | 16       | 0.16          |
| (1,168) | 1:27:A:ILE:HA   | 1:29:A:THR:H    | 18       | 0.16          |
| (1,144) | 1:30:A:SER:H    | 1:30:A:SER:HB2  | 12       | 0.16          |
| (1,88)  | 1:41:A:GLU:HA   | 1:45:A:ARG:H    | 14       | 0.16          |
| (1,36)  | 1:11:A:LYS:H    | 1:12:A:LYS:H    | 11       | 0.16          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB2  | 19       | 0.16          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 19       | 0.16          |
| (2,37)  | 1:48:A:LYS:H    | 1:44:A:HIS:O    | 13       | 0.15          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 13       | 0.15          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 18       | 0.15          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 19       | 0.15          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 10       | 0.15          |
| (2,31)  | 1:44:A:HIS:H    | 1:40:A:ARG:O    | 11       | 0.15          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 3        | 0.15          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 6        | 0.15          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 14       | 0.15          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 16       | 0.15          |
| (2,12)  | 1:28:A:ASN:N    | 1:24:A:ARG:O    | 5        | 0.15          |
| (2,4)   | 1:24:A:ARG:N    | 1:20:A:TYR:O    | 6        | 0.15          |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 4        | 0.15          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 12       | 0.15          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD2  | 6        | 0.15          |
| (1,715) | 1:27:A:ILE:HG21 | 1:40:A:ARG:HD3  | 6        | 0.15          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD2  | 6        | 0.15          |
| (1,715) | 1:27:A:ILE:HG22 | 1:40:A:ARG:HD3  | 6        | 0.15          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD2  | 6        | 0.15          |
| (1,715) | 1:27:A:ILE:HG23 | 1:40:A:ARG:HD3  | 6        | 0.15          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 8        | 0.15          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 8        | 0.15          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 8        | 0.15          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 1        | 0.15          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 1        | 0.15          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 1        | 0.15          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 15       | 0.15          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 15       | 0.15          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 15       | 0.15          |
| (1,554) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD21 | 13       | 0.15          |
| (1,554) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD22 | 13       | 0.15          |
| (1,554) | 1:30:A:SER:HB3  | 1:35:A:LEU:HD23 | 13       | 0.15          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD21 | 10       | 0.15          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD22 | 10       | 0.15          |
| (1,447) | 1:13:A:TYR:HE1  | 1:35:A:LEU:HD23 | 10       | 0.15          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD21 | 10       | 0.15          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD22 | 10       | 0.15          |
| (1,447) | 1:13:A:TYR:HE2  | 1:35:A:LEU:HD23 | 10       | 0.15          |
| (1,392) | 1:18:A:TRP:HZ3  | 1:23:A:LEU:HA   | 4        | 0.15          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 6        | 0.15          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 6        | 0.15          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 12       | 0.15          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 12       | 0.15          |
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 20       | 0.15          |
| (1,275) | 1:44:A:HIS:H    | 1:47:A:LEU:HB2  | 6        | 0.15          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 9        | 0.15          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 9        | 0.15          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 9        | 0.15          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 15       | 0.15          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 15       | 0.15          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 15       | 0.15          |
| (1,247) | 1:34:A:GLU:HB2  | 1:37:A:ALA:H    | 3        | 0.15          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 1        | 0.15          |
| (1,148) | 1:15:A:LEU:H    | 1:16:A:SER:H    | 18       | 0.15          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,20)  | 1:35:A:LEU:H   | 1:38:A:ALA:HB1  | 17       | 0.15          |
| (1,20)  | 1:35:A:LEU:H   | 1:38:A:ALA:HB2  | 17       | 0.15          |
| (1,20)  | 1:35:A:LEU:H   | 1:38:A:ALA:HB3  | 17       | 0.15          |
| (2,29)  | 1:43:A:PHE:H   | 1:39:A:CYS:O    | 4        | 0.14          |
| (2,29)  | 1:43:A:PHE:H   | 1:39:A:CYS:O    | 15       | 0.14          |
| (2,28)  | 1:42:A:GLU:N   | 1:38:A:ALA:O    | 3        | 0.14          |
| (2,26)  | 1:41:A:GLU:N   | 1:37:A:ALA:O    | 11       | 0.14          |
| (2,25)  | 1:41:A:GLU:H   | 1:37:A:ALA:O    | 10       | 0.14          |
| (2,18)  | 1:37:A:ALA:N   | 1:33:A:ILE:O    | 18       | 0.14          |
| (2,18)  | 1:37:A:ALA:N   | 1:33:A:ILE:O    | 20       | 0.14          |
| (2,10)  | 1:27:A:ILE:N   | 1:23:A:LEU:O    | 3        | 0.14          |
| (2,10)  | 1:27:A:ILE:N   | 1:23:A:LEU:O    | 6        | 0.14          |
| (2,10)  | 1:27:A:ILE:N   | 1:23:A:LEU:O    | 15       | 0.14          |
| (2,9)   | 1:27:A:ILE:H   | 1:23:A:LEU:O    | 4        | 0.14          |
| (2,7)   | 1:26:A:THR:H   | 1:22:A:GLU:O    | 20       | 0.14          |
| (2,3)   | 1:24:A:ARG:H   | 1:20:A:TYR:O    | 3        | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD11 | 3        | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD12 | 3        | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD13 | 3        | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD21 | 3        | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD22 | 3        | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD23 | 3        | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD11 | 18       | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD12 | 18       | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD13 | 18       | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD21 | 18       | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD22 | 18       | 0.14          |
| (1,787) | 1:46:A:ARG:H   | 1:47:A:LEU:HD23 | 18       | 0.14          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD11 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD12 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD13 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD21 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD22 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB2 | 1:47:A:LEU:HD23 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD11 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD12 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD13 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD21 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD22 | 14       | 0.14          |
| (1,765) | 1:43:A:PHE:HB3 | 1:47:A:LEU:HD23 | 14       | 0.14          |
| (1,761) | 1:43:A:PHE:H   | 1:44:A:HIS:HB2  | 18       | 0.14          |
| (1,761) | 1:43:A:PHE:H   | 1:44:A:HIS:HB3  | 18       | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 14       | 0.14          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 14       | 0.14          |
| (1,728) | 1:34:A:GLU:HG2  | 1:35:A:LEU:H    | 18       | 0.14          |
| (1,728) | 1:34:A:GLU:HG3  | 1:35:A:LEU:H    | 18       | 0.14          |
| (1,725) | 1:33:A:ILE:HG21 | 1:34:A:GLU:HG2  | 18       | 0.14          |
| (1,725) | 1:33:A:ILE:HG21 | 1:34:A:GLU:HG3  | 18       | 0.14          |
| (1,725) | 1:33:A:ILE:HG22 | 1:34:A:GLU:HG2  | 18       | 0.14          |
| (1,725) | 1:33:A:ILE:HG22 | 1:34:A:GLU:HG3  | 18       | 0.14          |
| (1,725) | 1:33:A:ILE:HG23 | 1:34:A:GLU:HG2  | 18       | 0.14          |
| (1,725) | 1:33:A:ILE:HG23 | 1:34:A:GLU:HG3  | 18       | 0.14          |
| (1,640) | 1:19:A:LYS:HA   | 1:19:A:LYS:HD3  | 4        | 0.14          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 9        | 0.14          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 9        | 0.14          |
| (1,590) | 1:27:A:ILE:HA   | 1:36:A:LEU:HG   | 16       | 0.14          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 8        | 0.14          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 8        | 0.14          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD11 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD12 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD13 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD11 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD12 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD13 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD11 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD12 | 8        | 0.14          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD13 | 8        | 0.14          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 5        | 0.14          |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 5        | 0.14          |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 5        | 0.14          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD21 | 16       | 0.14          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD22 | 16       | 0.14          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD23 | 16       | 0.14          |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB2  | 4        | 0.14          |
| (1,362) | 1:10:A:THR:HA   | 1:11:A:LYS:HB3  | 4        | 0.14          |
| (1,325) | 1:27:A:ILE:HD11 | 1:40:A:ARG:HA   | 9        | 0.14          |
| (1,325) | 1:27:A:ILE:HD12 | 1:40:A:ARG:HA   | 9        | 0.14          |
| (1,325) | 1:27:A:ILE:HD13 | 1:40:A:ARG:HA   | 9        | 0.14          |
| (1,319) | 1:43:A:PHE:HB3  | 1:46:A:ARG:H    | 3        | 0.14          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD21 | 6        | 0.14          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD22 | 6        | 0.14          |
| (1,316) | 1:18:A:TRP:HE1  | 1:23:A:LEU:HD23 | 6        | 0.14          |
| (1,298) | 1:43:A:PHE:HD1  | 1:46:A:ARG:H    | 17       | 0.14          |
| (1,298) | 1:43:A:PHE:HD2  | 1:46:A:ARG:H    | 17       | 0.14          |
| (1,273) | 1:27:A:ILE:HD11 | 1:43:A:PHE:H    | 20       | 0.14          |
| (1,273) | 1:27:A:ILE:HD12 | 1:43:A:PHE:H    | 20       | 0.14          |
| (1,273) | 1:27:A:ILE:HD13 | 1:43:A:PHE:H    | 20       | 0.14          |
| (1,268) | 1:38:A:ALA:H    | 1:41:A:GLU:H    | 14       | 0.14          |
| (1,268) | 1:38:A:ALA:H    | 1:41:A:GLU:H    | 19       | 0.14          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 17       | 0.14          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 17       | 0.14          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 17       | 0.14          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 18       | 0.14          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 18       | 0.14          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 18       | 0.14          |
| (1,170) | 1:28:A:ASN:HB2  | 1:30:A:SER:H    | 10       | 0.14          |
| (1,170) | 1:28:A:ASN:HB2  | 1:30:A:SER:H    | 20       | 0.14          |
| (1,148) | 1:15:A:LEU:H    | 1:16:A:SER:H    | 3        | 0.14          |
| (1,148) | 1:15:A:LEU:H    | 1:16:A:SER:H    | 17       | 0.14          |
| (1,140) | 1:29:A:THR:H    | 1:30:A:SER:H    | 16       | 0.14          |
| (1,91)  | 1:34:A:GLU:HA   | 1:37:A:ALA:H    | 13       | 0.14          |
| (1,41)  | 1:2:A:PRO:HA    | 1:3:A:LEU:H     | 10       | 0.14          |
| (1,41)  | 1:2:A:PRO:HA    | 1:3:A:LEU:H     | 16       | 0.14          |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 2        | 0.14          |
| (2,37)  | 1:48:A:LYS:H    | 1:44:A:HIS:O    | 12       | 0.13          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 2        | 0.13          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 7        | 0.13          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 12       | 0.13          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 16       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,19)  | 1:38:A:ALA:H    | 1:34:A:GLU:O    | 9        | 0.13          |
| (2,19)  | 1:38:A:ALA:H    | 1:34:A:GLU:O    | 14       | 0.13          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 9        | 0.13          |
| (2,12)  | 1:28:A:ASN:N    | 1:24:A:ARG:O    | 11       | 0.13          |
| (2,4)   | 1:24:A:ARG:N    | 1:20:A:TYR:O    | 4        | 0.13          |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 6        | 0.13          |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 7        | 0.13          |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 17       | 0.13          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 5        | 0.13          |
| (2,1)   | 1:23:A:LEU:H    | 1:19:A:LYS:O    | 9        | 0.13          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD11 | 8        | 0.13          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD12 | 8        | 0.13          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD13 | 8        | 0.13          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD21 | 8        | 0.13          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD22 | 8        | 0.13          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD23 | 8        | 0.13          |
| (1,750) | 1:40:A:ARG:HD2  | 1:41:A:GLU:H    | 12       | 0.13          |
| (1,750) | 1:40:A:ARG:HD3  | 1:41:A:GLU:H    | 12       | 0.13          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 7        | 0.13          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 7        | 0.13          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 16       | 0.13          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 16       | 0.13          |
| (1,665) | 1:12:A:LYS:HG2  | 1:13:A:TYR:H    | 2        | 0.13          |
| (1,665) | 1:12:A:LYS:HG3  | 1:13:A:TYR:H    | 2        | 0.13          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 17       | 0.13          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 17       | 0.13          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 17       | 0.13          |
| (1,634) | 1:29:A:THR:H    | 1:30:A:SER:HB3  | 13       | 0.13          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 10       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 10       | 0.13          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 18       | 0.13          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 18       | 0.13          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 17       | 0.13          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 17       | 0.13          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 17       | 0.13          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 19       | 0.13          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 19       | 0.13          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 19       | 0.13          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD11 | 1        | 0.13          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD12 | 1        | 0.13          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD13 | 1        | 0.13          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD11 | 1        | 0.13          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD12 | 1        | 0.13          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD13 | 1        | 0.13          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD11 | 1        | 0.13          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD12 | 1        | 0.13          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD13 | 1        | 0.13          |
| (1,509) | 1:19:A:LYS:HA   | 1:19:A:LYS:HD2  | 18       | 0.13          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 13       | 0.13          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 13       | 0.13          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 13       | 0.13          |
| (1,292) | 1:27:A:ILE:HG12 | 1:39:A:CYS:H    | 14       | 0.13          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,290) | 1:28:A:ASN:H    | 1:30:A:SER:H    | 1        | 0.13          |
| (1,279) | 1:44:A:HIS:HD2  | 1:45:A:ARG:H    | 10       | 0.13          |
| (1,268) | 1:38:A:ALA:H    | 1:41:A:GLU:H    | 7        | 0.13          |
| (1,255) | 1:23:A:LEU:HD21 | 1:39:A:CYS:H    | 10       | 0.13          |
| (1,255) | 1:23:A:LEU:HD22 | 1:39:A:CYS:H    | 10       | 0.13          |
| (1,255) | 1:23:A:LEU:HD23 | 1:39:A:CYS:H    | 10       | 0.13          |
| (1,249) | 1:15:A:LEU:HD11 | 1:38:A:ALA:H    | 20       | 0.13          |
| (1,249) | 1:15:A:LEU:HD12 | 1:38:A:ALA:H    | 20       | 0.13          |
| (1,249) | 1:15:A:LEU:HD13 | 1:38:A:ALA:H    | 20       | 0.13          |
| (1,226) | 1:26:A:THR:HG21 | 1:31:A:CYS:H    | 6        | 0.13          |
| (1,226) | 1:26:A:THR:HG22 | 1:31:A:CYS:H    | 6        | 0.13          |
| (1,226) | 1:26:A:THR:HG23 | 1:31:A:CYS:H    | 6        | 0.13          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 16       | 0.13          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 16       | 0.13          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 16       | 0.13          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 9        | 0.13          |
| (1,197) | 1:18:A:TRP:HB3  | 1:22:A:GLU:H    | 2        | 0.13          |
| (1,161) | 1:10:A:THR:H    | 1:11:A:LYS:H    | 12       | 0.13          |
| (1,148) | 1:15:A:LEU:H    | 1:16:A:SER:H    | 8        | 0.13          |
| (1,148) | 1:15:A:LEU:H    | 1:16:A:SER:H    | 11       | 0.13          |
| (1,144) | 1:30:A:SER:H    | 1:30:A:SER:HB2  | 6        | 0.13          |
| (1,110) | 1:49:A:VAL:H    | 1:49:A:VAL:HB   | 17       | 0.13          |
| (1,101) | 1:41:A:GLU:H    | 1:41:A:GLU:HG3  | 10       | 0.13          |
| (1,41)  | 1:2:A:PRO:HA    | 1:3:A:LEU:H     | 3        | 0.13          |
| (1,41)  | 1:2:A:PRO:HA    | 1:3:A:LEU:H     | 17       | 0.13          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB2  | 17       | 0.13          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 17       | 0.13          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB1  | 3        | 0.13          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB2  | 3        | 0.13          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB3  | 3        | 0.13          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB1  | 18       | 0.13          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB2  | 18       | 0.13          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB3  | 18       | 0.13          |
| (1,10)  | 1:50:A:TYR:H    | 1:51:A:HIS:H    | 16       | 0.13          |
| (2,40)  | 1:49:A:VAL:N    | 1:45:A:ARG:O    | 6        | 0.12          |
| (2,34)  | 1:45:A:ARG:N    | 1:41:A:GLU:O    | 13       | 0.12          |
| (2,33)  | 1:45:A:ARG:H    | 1:41:A:GLU:O    | 1        | 0.12          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 11       | 0.12          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 7        | 0.12          |
| (2,26)  | 1:41:A:GLU:N    | 1:37:A:ALA:O    | 4        | 0.12          |
| (2,26)  | 1:41:A:GLU:N    | 1:37:A:ALA:O    | 5        | 0.12          |
| (2,26)  | 1:41:A:GLU:N    | 1:37:A:ALA:O    | 14       | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,26)  | 1:41:A:GLU:N    | 1:37:A:ALA:O    | 20       | 0.12          |
| (2,25)  | 1:41:A:GLU:H    | 1:37:A:ALA:O    | 1        | 0.12          |
| (2,19)  | 1:38:A:ALA:H    | 1:34:A:GLU:O    | 13       | 0.12          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 7        | 0.12          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 11       | 0.12          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 19       | 0.12          |
| (2,12)  | 1:28:A:ASN:N    | 1:24:A:ARG:O    | 1        | 0.12          |
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 2        | 0.12          |
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 17       | 0.12          |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 2        | 0.12          |
| (2,2)   | 1:23:A:LEU:N    | 1:19:A:LYS:O    | 15       | 0.12          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD11 | 12       | 0.12          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD12 | 12       | 0.12          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD13 | 12       | 0.12          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD21 | 12       | 0.12          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD22 | 12       | 0.12          |
| (1,787) | 1:46:A:ARG:H    | 1:47:A:LEU:HD23 | 12       | 0.12          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 4        | 0.12          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 4        | 0.12          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 13       | 0.12          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 13       | 0.12          |
| (1,685) | 1:19:A:LYS:H    | 1:19:A:LYS:HD2  | 4        | 0.12          |
| (1,685) | 1:19:A:LYS:H    | 1:19:A:LYS:HD3  | 4        | 0.12          |
| (1,647) | 1:34:A:GLU:HB2  | 1:35:A:LEU:HG   | 17       | 0.12          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 5        | 0.12          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 5        | 0.12          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 5        | 0.12          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 18       | 0.12          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 18       | 0.12          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 18       | 0.12          |
| (1,634) | 1:29:A:THR:H    | 1:30:A:SER:HB3  | 9        | 0.12          |
| (1,634) | 1:29:A:THR:H    | 1:30:A:SER:HB3  | 20       | 0.12          |
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 5        | 0.12          |
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 13       | 0.12          |
| (1,627) | 1:13:A:TYR:HA   | 1:15:A:LEU:HD21 | 13       | 0.12          |
| (1,627) | 1:13:A:TYR:HA   | 1:15:A:LEU:HD22 | 13       | 0.12          |
| (1,627) | 1:13:A:TYR:HA   | 1:15:A:LEU:HD23 | 13       | 0.12          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD21 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD22 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD21 | 1:23:A:LEU:HD23 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD21 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD22 | 4        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,599) | 1:15:A:LEU:HD22 | 1:23:A:LEU:HD23 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD21 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD22 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD23 | 1:23:A:LEU:HD23 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD21 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD22 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD11 | 1:23:A:LEU:HD23 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD21 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD22 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD12 | 1:23:A:LEU:HD23 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD21 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD22 | 4        | 0.12          |
| (1,599) | 1:15:A:LEU:HD13 | 1:23:A:LEU:HD23 | 4        | 0.12          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 3        | 0.12          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 5        | 0.12          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 12       | 0.12          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 12       | 0.12          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 12       | 0.12          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD11 | 10       | 0.12          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD12 | 10       | 0.12          |
| (1,549) | 1:15:A:LEU:HD21 | 1:35:A:LEU:HD13 | 10       | 0.12          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD11 | 10       | 0.12          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD12 | 10       | 0.12          |
| (1,549) | 1:15:A:LEU:HD22 | 1:35:A:LEU:HD13 | 10       | 0.12          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD11 | 10       | 0.12          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD12 | 10       | 0.12          |
| (1,549) | 1:15:A:LEU:HD23 | 1:35:A:LEU:HD13 | 10       | 0.12          |
| (1,534) | 1:44:A:HIS:HA   | 1:44:A:HIS:HD2  | 1        | 0.12          |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 2        | 0.12          |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 2        | 0.12          |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 2        | 0.12          |
| (1,525) | 1:35:A:LEU:HD21 | 1:39:A:CYS:H    | 11       | 0.12          |
| (1,525) | 1:35:A:LEU:HD22 | 1:39:A:CYS:H    | 11       | 0.12          |
| (1,525) | 1:35:A:LEU:HD23 | 1:39:A:CYS:H    | 11       | 0.12          |
| (1,488) | 1:26:A:THR:HG21 | 1:30:A:SER:HA   | 8        | 0.12          |
| (1,488) | 1:26:A:THR:HG22 | 1:30:A:SER:HA   | 8        | 0.12          |
| (1,488) | 1:26:A:THR:HG23 | 1:30:A:SER:HA   | 8        | 0.12          |
| (1,463) | 1:15:A:LEU:HD21 | 1:18:A:TRP:HE3  | 11       | 0.12          |
| (1,463) | 1:15:A:LEU:HD22 | 1:18:A:TRP:HE3  | 11       | 0.12          |
| (1,463) | 1:15:A:LEU:HD23 | 1:18:A:TRP:HE3  | 11       | 0.12          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD21 | 5        | 0.12          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD22 | 5        | 0.12          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD23 | 5        | 0.12          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD21 | 2        | 0.12          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD22 | 2        | 0.12          |
| (1,420) | 1:18:A:TRP:HE3  | 1:23:A:LEU:HD23 | 2        | 0.12          |
| (1,419) | 1:23:A:LEU:H    | 1:23:A:LEU:HD21 | 13       | 0.12          |
| (1,419) | 1:23:A:LEU:H    | 1:23:A:LEU:HD22 | 13       | 0.12          |
| (1,419) | 1:23:A:LEU:H    | 1:23:A:LEU:HD23 | 13       | 0.12          |
| (1,361) | 1:49:A:VAL:HA   | 1:50:A:TYR:H    | 2        | 0.12          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 2        | 0.12          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 2        | 0.12          |
| (1,348) | 1:41:A:GLU:H    | 1:41:A:GLU:HG2  | 10       | 0.12          |
| (1,309) | 1:22:A:GLU:H    | 1:23:A:LEU:HG   | 13       | 0.12          |
| (1,301) | 1:17:A:LYS:H    | 1:18:A:TRP:HB2  | 9        | 0.12          |
| (1,288) | 1:24:A:ARG:HG2  | 1:28:A:ASN:HD21 | 5        | 0.12          |
| (1,277) | 1:44:A:HIS:H    | 1:44:A:HIS:HD2  | 17       | 0.12          |
| (1,268) | 1:38:A:ALA:H    | 1:41:A:GLU:H    | 13       | 0.12          |
| (1,250) | 1:35:A:LEU:HD21 | 1:38:A:ALA:H    | 15       | 0.12          |
| (1,250) | 1:35:A:LEU:HD22 | 1:38:A:ALA:H    | 15       | 0.12          |
| (1,250) | 1:35:A:LEU:HD23 | 1:38:A:ALA:H    | 15       | 0.12          |
| (1,241) | 1:13:A:TYR:HE1  | 1:35:A:LEU:H    | 14       | 0.12          |
| (1,241) | 1:13:A:TYR:HE2  | 1:35:A:LEU:H    | 14       | 0.12          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD21 | 13       | 0.12          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD22 | 13       | 0.12          |
| (1,211) | 1:18:A:TRP:H    | 1:23:A:LEU:HD23 | 13       | 0.12          |
| (1,207) | 1:18:A:TRP:HD1  | 1:19:A:LYS:H    | 10       | 0.12          |
| (1,199) | 1:19:A:LYS:HA   | 1:21:A:ALA:H    | 8        | 0.12          |
| (1,109) | 1:49:A:VAL:H    | 1:50:A:TYR:H    | 4        | 0.12          |
| (1,91)  | 1:34:A:GLU:HA   | 1:37:A:ALA:H    | 9        | 0.12          |
| (1,91)  | 1:34:A:GLU:HA   | 1:37:A:ALA:H    | 16       | 0.12          |
| (1,91)  | 1:34:A:GLU:HA   | 1:37:A:ALA:H    | 18       | 0.12          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB2  | 5        | 0.12          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 5        | 0.12          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB2  | 18       | 0.12          |
| (1,27)  | 1:11:A:LYS:H    | 1:11:A:LYS:HB3  | 18       | 0.12          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB1  | 16       | 0.12          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB2  | 16       | 0.12          |
| (1,20)  | 1:35:A:LEU:H    | 1:38:A:ALA:HB3  | 16       | 0.12          |
| (2,38)  | 1:48:A:LYS:N    | 1:44:A:HIS:O    | 13       | 0.11          |
| (2,32)  | 1:44:A:HIS:N    | 1:40:A:ARG:O    | 10       | 0.11          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 1        | 0.11          |
| (2,29)  | 1:43:A:PHE:H    | 1:39:A:CYS:O    | 13       | 0.11          |
| (2,27)  | 1:42:A:GLU:H    | 1:38:A:ALA:O    | 9        | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,26)  | 1:41:A:GLU:N    | 1:37:A:ALA:O    | 17       | 0.11          |
| (2,24)  | 1:40:A:ARG:N    | 1:36:A:LEU:O    | 10       | 0.11          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 2        | 0.11          |
| (2,18)  | 1:37:A:ALA:N    | 1:33:A:ILE:O    | 4        | 0.11          |
| (2,12)  | 1:28:A:ASN:N    | 1:24:A:ARG:O    | 6        | 0.11          |
| (2,11)  | 1:28:A:ASN:H    | 1:24:A:ARG:O    | 9        | 0.11          |
| (2,10)  | 1:27:A:ILE:N    | 1:23:A:LEU:O    | 8        | 0.11          |
| (2,10)  | 1:27:A:ILE:N    | 1:23:A:LEU:O    | 9        | 0.11          |
| (2,9)   | 1:27:A:ILE:H    | 1:23:A:LEU:O    | 20       | 0.11          |
| (2,6)   | 1:25:A:ASP:N    | 1:21:A:ALA:O    | 17       | 0.11          |
| (2,3)   | 1:24:A:ARG:H    | 1:20:A:TYR:O    | 11       | 0.11          |
| (1,804) | 1:49:A:VAL:HG11 | 1:50:A:TYR:HD1  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG11 | 1:50:A:TYR:HD2  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG12 | 1:50:A:TYR:HD1  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG12 | 1:50:A:TYR:HD2  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG13 | 1:50:A:TYR:HD1  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG13 | 1:50:A:TYR:HD2  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG21 | 1:50:A:TYR:HD1  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG21 | 1:50:A:TYR:HD2  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG22 | 1:50:A:TYR:HD1  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG22 | 1:50:A:TYR:HD2  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG23 | 1:50:A:TYR:HD1  | 14       | 0.11          |
| (1,804) | 1:49:A:VAL:HG23 | 1:50:A:TYR:HD2  | 14       | 0.11          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG11 | 2        | 0.11          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG12 | 2        | 0.11          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG13 | 2        | 0.11          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG21 | 2        | 0.11          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG22 | 2        | 0.11          |
| (1,790) | 1:46:A:ARG:HA   | 1:49:A:VAL:HG23 | 2        | 0.11          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB2  | 3        | 0.11          |
| (1,740) | 1:39:A:CYS:HA   | 1:42:A:GLU:HB3  | 3        | 0.11          |
| (1,731) | 1:37:A:ALA:HA   | 1:40:A:ARG:HD2  | 16       | 0.11          |
| (1,731) | 1:37:A:ALA:HA   | 1:40:A:ARG:HD3  | 16       | 0.11          |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE1  | 7        | 0.11          |
| (1,712) | 1:24:A:ARG:HD2  | 1:43:A:PHE:HE2  | 7        | 0.11          |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE1  | 7        | 0.11          |
| (1,712) | 1:24:A:ARG:HD3  | 1:43:A:PHE:HE2  | 7        | 0.11          |
| (1,644) | 1:48:A:LYS:HD2  | 1:49:A:VAL:H    | 16       | 0.11          |
| (1,644) | 1:48:A:LYS:HD3  | 1:49:A:VAL:H    | 16       | 0.11          |
| (1,636) | 1:15:A:LEU:HD11 | 1:18:A:TRP:HE3  | 10       | 0.11          |
| (1,636) | 1:15:A:LEU:HD12 | 1:18:A:TRP:HE3  | 10       | 0.11          |
| (1,636) | 1:15:A:LEU:HD13 | 1:18:A:TRP:HE3  | 10       | 0.11          |

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| Key     | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,631) | 1:10:A:THR:HB   | 1:11:A:LYS:H    | 11       | 0.11          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 8        | 0.11          |
| (1,584) | 1:43:A:PHE:HA   | 1:46:A:ARG:HD3  | 11       | 0.11          |
| (1,570) | 1:23:A:LEU:HD11 | 1:39:A:CYS:HA   | 13       | 0.11          |
| (1,570) | 1:23:A:LEU:HD12 | 1:39:A:CYS:HA   | 13       | 0.11          |
| (1,570) | 1:23:A:LEU:HD13 | 1:39:A:CYS:HA   | 13       | 0.11          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD21 | 4        | 0.11          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD22 | 4        | 0.11          |
| (1,565) | 1:30:A:SER:HB3  | 1:36:A:LEU:HD23 | 4        | 0.11          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD21 | 15       | 0.11          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD22 | 15       | 0.11          |
| (1,553) | 1:18:A:TRP:HZ2  | 1:35:A:LEU:HD23 | 15       | 0.11          |
| (1,509) | 1:19:A:LYS:HA   | 1:19:A:LYS:HD2  | 12       | 0.11          |
| (1,508) | 1:19:A:LYS:H    | 1:19:A:LYS:HG3  | 16       | 0.11          |
| (1,463) | 1:15:A:LEU:HD21 | 1:18:A:TRP:HE3  | 5        | 0.11          |
| (1,463) | 1:15:A:LEU:HD22 | 1:18:A:TRP:HE3  | 5        | 0.11          |
| (1,463) | 1:15:A:LEU:HD23 | 1:18:A:TRP:HE3  | 5        | 0.11          |
| (1,463) | 1:15:A:LEU:HD21 | 1:18:A:TRP:HE3  | 17       | 0.11          |
| (1,463) | 1:15:A:LEU:HD22 | 1:18:A:TRP:HE3  | 17       | 0.11          |
| (1,463) | 1:15:A:LEU:HD23 | 1:18:A:TRP:HE3  | 17       | 0.11          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD21 | 3        | 0.11          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD22 | 3        | 0.11          |
| (1,446) | 1:18:A:TRP:HH2  | 1:35:A:LEU:HD23 | 3        | 0.11          |
| (1,445) | 1:28:A:ASN:HA   | 1:28:A:ASN:HD22 | 2        | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD21 | 7        | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD22 | 7        | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD23 | 7        | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD21 | 8        | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD22 | 8        | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD23 | 8        | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD21 | 15       | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD22 | 15       | 0.11          |
| (1,434) | 1:47:A:LEU:H    | 1:47:A:LEU:HD23 | 15       | 0.11          |
| (1,392) | 1:18:A:TRP:HZ3  | 1:23:A:LEU:HA   | 1        | 0.11          |
| (1,354) | 1:48:A:LYS:HB2  | 1:49:A:VAL:HA   | 5        | 0.11          |
| (1,354) | 1:48:A:LYS:HB3  | 1:49:A:VAL:HA   | 5        | 0.11          |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB1  | 18       | 0.11          |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB2  | 18       | 0.11          |
| (1,340) | 1:13:A:TYR:HB2  | 1:38:A:ALA:HB3  | 18       | 0.11          |
| (1,254) | 1:15:A:LEU:HD11 | 1:39:A:CYS:H    | 12       | 0.11          |
| (1,254) | 1:15:A:LEU:HD12 | 1:39:A:CYS:H    | 12       | 0.11          |
| (1,254) | 1:15:A:LEU:HD13 | 1:39:A:CYS:H    | 12       | 0.11          |

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| Key     | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,222) | 1:13:A:TYR:H   | 1:13:A:TYR:HE1  | 20       | 0.11          |
| (1,222) | 1:13:A:TYR:H   | 1:13:A:TYR:HE2  | 20       | 0.11          |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD21 | 9        | 0.11          |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD22 | 9        | 0.11          |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD23 | 9        | 0.11          |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD21 | 11       | 0.11          |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD22 | 11       | 0.11          |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD23 | 11       | 0.11          |
| (1,170) | 1:28:A:ASN:HB2 | 1:30:A:SER:H    | 1        | 0.11          |
| (1,148) | 1:15:A:LEU:H   | 1:16:A:SER:H    | 1        | 0.11          |
| (1,148) | 1:15:A:LEU:H   | 1:16:A:SER:H    | 4        | 0.11          |
| (1,109) | 1:49:A:VAL:H   | 1:50:A:TYR:H    | 18       | 0.11          |
| (1,101) | 1:41:A:GLU:H   | 1:41:A:GLU:HG3  | 6        | 0.11          |
| (1,88)  | 1:41:A:GLU:HA  | 1:45:A:ARG:H    | 4        | 0.11          |
| (1,88)  | 1:41:A:GLU:HA  | 1:45:A:ARG:H    | 7        | 0.11          |
| (1,88)  | 1:41:A:GLU:HA  | 1:45:A:ARG:H    | 12       | 0.11          |
| (1,42)  | 1:3:A:LEU:H    | 1:3:A:LEU:HG    | 18       | 0.11          |
| (1,41)  | 1:2:A:PRO:HA   | 1:3:A:LEU:H     | 6        | 0.11          |
| (1,22)  | 1:35:A:LEU:H   | 1:35:A:LEU:HD11 | 17       | 0.11          |
| (1,22)  | 1:35:A:LEU:H   | 1:35:A:LEU:HD12 | 17       | 0.11          |
| (1,22)  | 1:35:A:LEU:H   | 1:35:A:LEU:HD13 | 17       | 0.11          |
| (1,22)  | 1:35:A:LEU:H   | 1:35:A:LEU:HD21 | 17       | 0.11          |
| (1,22)  | 1:35:A:LEU:H   | 1:35:A:LEU:HD22 | 17       | 0.11          |
| (1,22)  | 1:35:A:LEU:H   | 1:35:A:LEU:HD23 | 17       | 0.11          |
| (2,37)  | 1:48:A:LYS:H   | 1:44:A:HIS:O    | 6        | 0.1           |
| (2,20)  | 1:38:A:ALA:N   | 1:34:A:GLU:O    | 14       | 0.1           |
| (2,18)  | 1:37:A:ALA:N   | 1:33:A:ILE:O    | 1        | 0.1           |
| (1,565) | 1:30:A:SER:HB3 | 1:36:A:LEU:HD21 | 7        | 0.1           |
| (1,565) | 1:30:A:SER:HB3 | 1:36:A:LEU:HD22 | 7        | 0.1           |
| (1,565) | 1:30:A:SER:HB3 | 1:36:A:LEU:HD23 | 7        | 0.1           |
| (1,502) | 1:18:A:TRP:HB3 | 1:22:A:GLU:HB3  | 19       | 0.1           |
| (1,316) | 1:18:A:TRP:HE1 | 1:23:A:LEU:HD21 | 5        | 0.1           |
| (1,316) | 1:18:A:TRP:HE1 | 1:23:A:LEU:HD22 | 5        | 0.1           |
| (1,316) | 1:18:A:TRP:HE1 | 1:23:A:LEU:HD23 | 5        | 0.1           |
| (1,279) | 1:44:A:HIS:HD2 | 1:45:A:ARG:H    | 18       | 0.1           |
| (1,232) | 1:32:A:ASP:H   | 1:35:A:LEU:HB3  | 3        | 0.1           |
| (1,229) | 1:30:A:SER:HG  | 1:31:A:CYS:H    | 8        | 0.1           |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD21 | 4        | 0.1           |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD22 | 4        | 0.1           |
| (1,211) | 1:18:A:TRP:H   | 1:23:A:LEU:HD23 | 4        | 0.1           |
| (1,197) | 1:18:A:TRP:HB3 | 1:22:A:GLU:H    | 10       | 0.1           |
| (1,156) | 1:19:A:LYS:HB2 | 1:22:A:GLU:H    | 16       | 0.1           |

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| Key    | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|--------|---------------|--------------|----------|---------------|
| (1,26) | 1:10:A:THR:HA | 1:11:A:LYS:H | 3        | 0.1           |

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

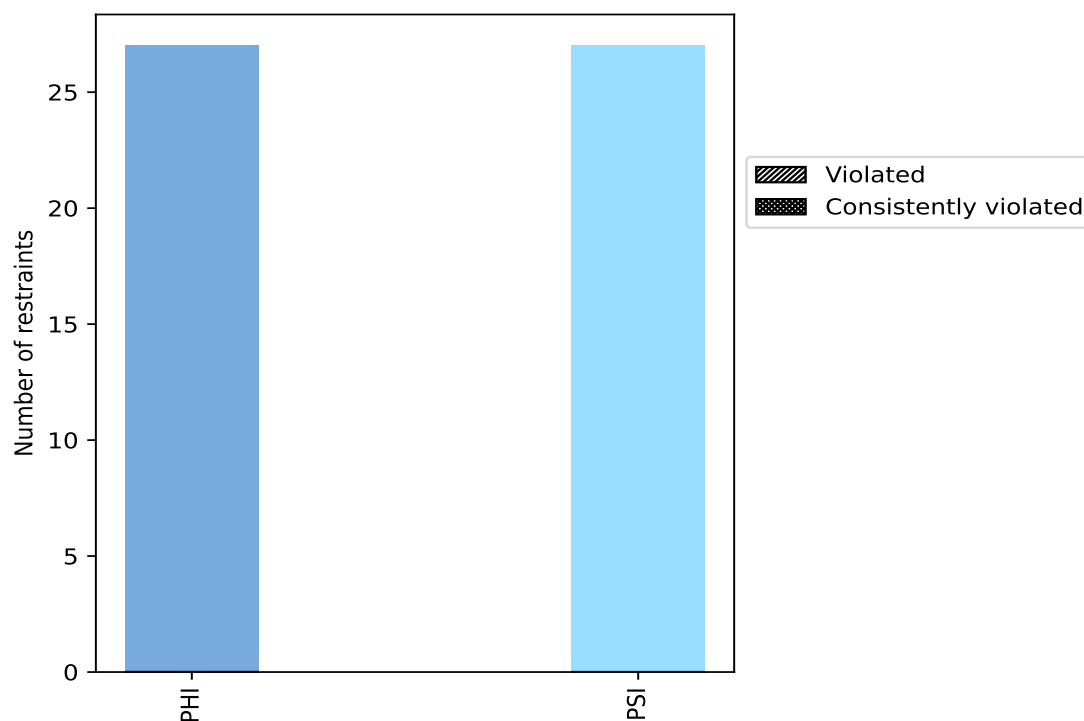
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PHI        | 27    | 50.0           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| PSI        | 27    | 50.0           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total      | 54    | 100.0          | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |

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

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



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

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

No violations found

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

No violations found

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

No violations found

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

No violations found