



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 12:12 AM UTC

PDB ID : 2MPF / pdb\_00002mpf  
BMRB ID : 19977  
Title : Solution structure human HCN2 CNBD in the cAMP-unbound state  
Authors : Saponaro, A.; Pauleta, S.R.; Cantini, F.; Matzapetakis, M.; Hammann, C.;  
Banci, L.; Thiel, G.; Santoro, B.; Moroni, A.  
Deposited on : 2014-05-16

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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

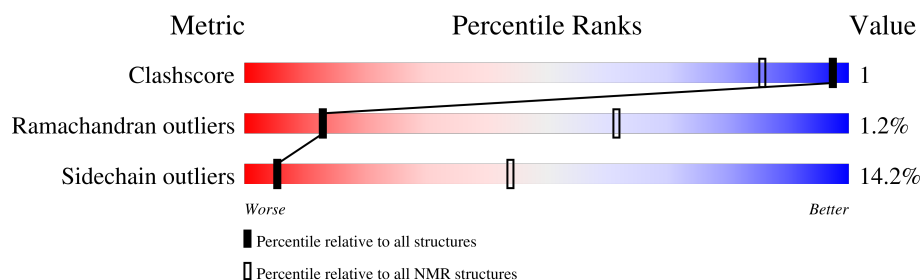
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 87%.

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     | 158    | <div> <div style="width: 65%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 11%; background-color: cyan;"></div> <div style="width: 12%; background-color: grey;"></div> </div> <div>65% 12% 11% 12%</div> |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:535-A:655 (121)     | 1.33              | 5            |

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 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2252 atoms, of which 1139 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 139      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2252  | 709 | 1139 | 195 | 200 | 9 |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 515     | GLY      | -      | expression tag | UNP Q9UL51 |
| A     | 516     | PRO      | -      | expression tag | UNP Q9UL51 |
| A     | 517     | SER      | -      | expression tag | UNP Q9UL51 |
| A     | 518     | SER      | -      | expression tag | UNP Q9UL51 |
| A     | 519     | PRO      | -      | expression tag | UNP Q9UL51 |
| A     | 520     | MET      | -      | expression tag | UNP Q9UL51 |

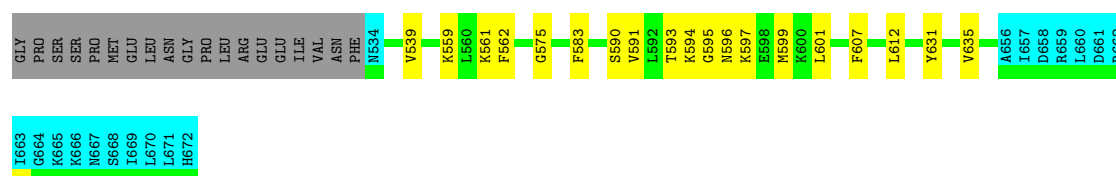
## 4 Residue-property plots [i](#)

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

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

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A: 



### 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

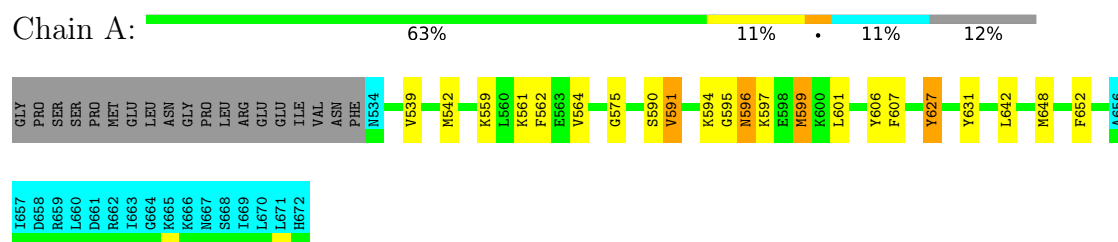
- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A: 



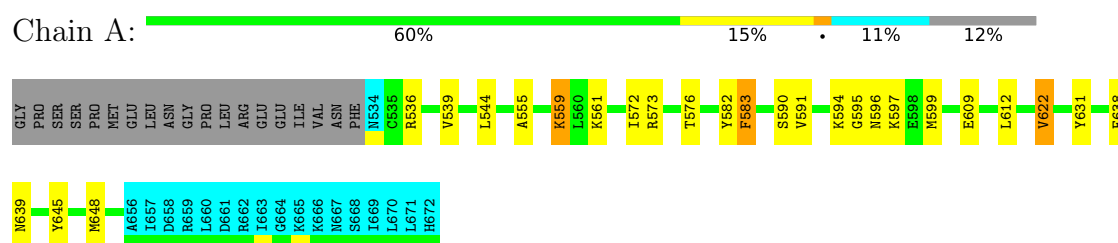
#### 4.2.2 Score per residue for model 2

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



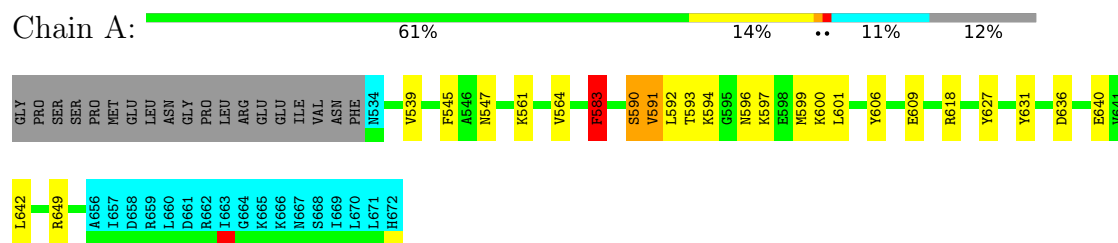
### 4.2.3 Score per residue for model 3

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



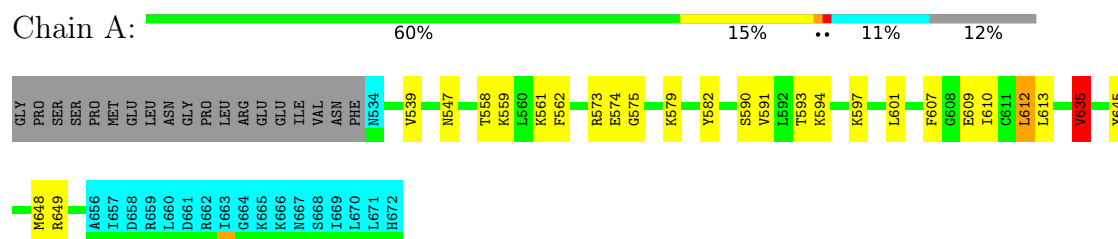
### 4.2.4 Score per residue for model 4

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



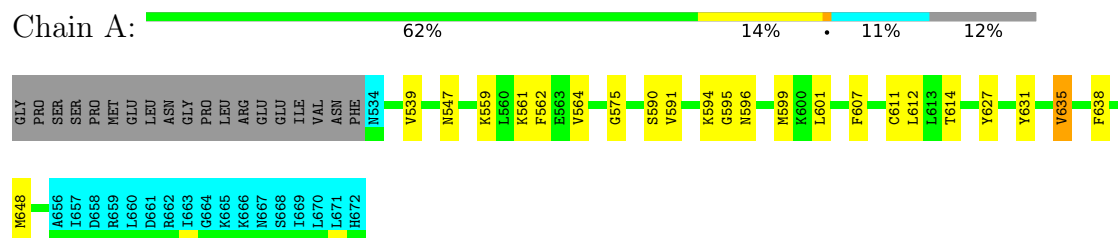
### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



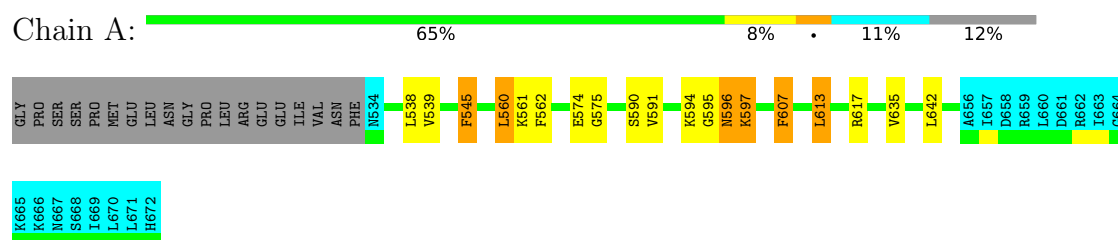
### 4.2.6 Score per residue for model 6

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



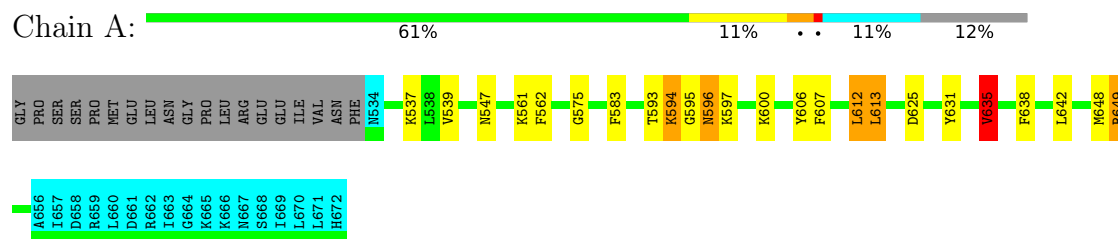
### 4.2.7 Score per residue for model 7

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



### 4.2.8 Score per residue for model 8

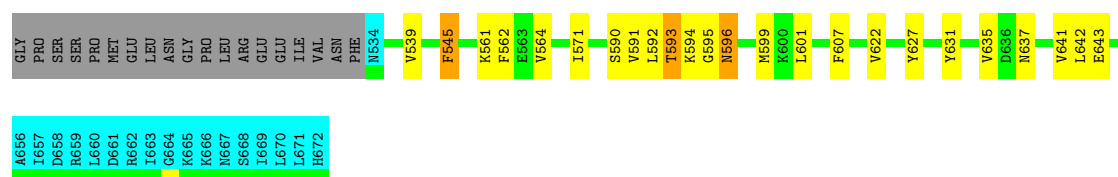
- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



### 4.2.9 Score per residue for model 9

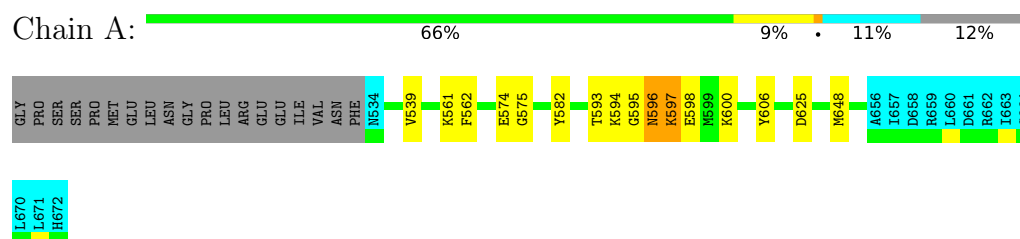
- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2





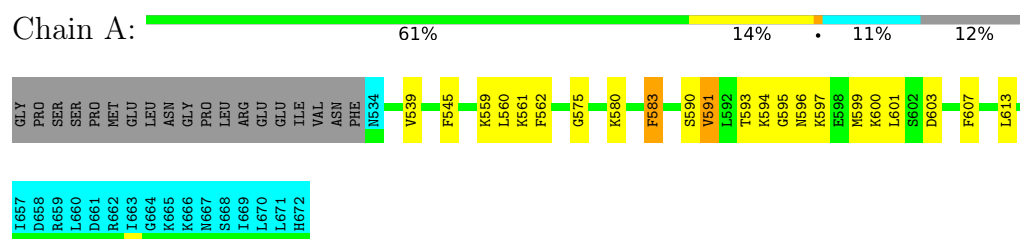
#### 4.2.10 Score per residue for model 10

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



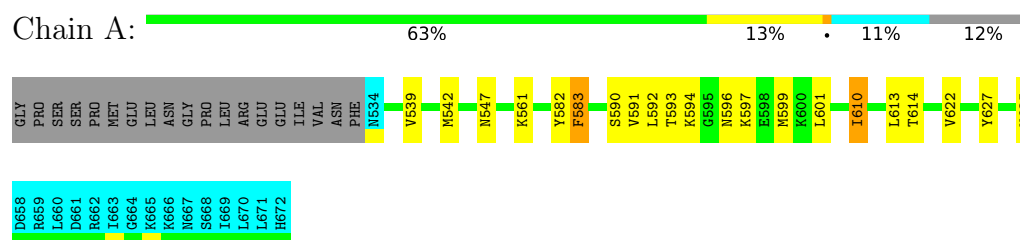
#### 4.2.11 Score per residue for model 11

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



#### 4.2.12 Score per residue for model 12

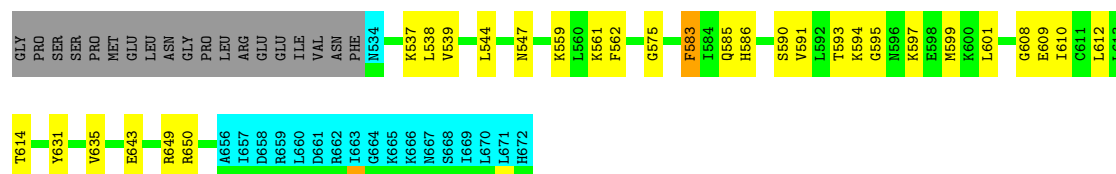
- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



### 4.2.13 Score per residue for model 13

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A: 



### 4.2.14 Score per residue for model 14

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

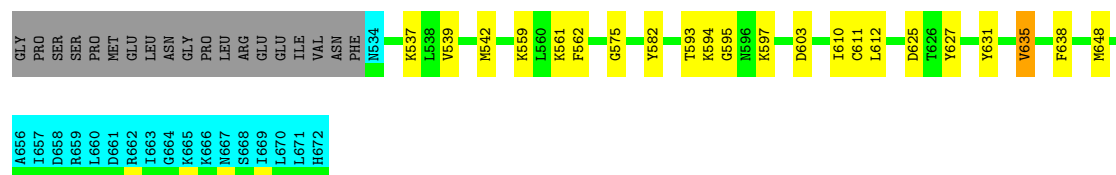
Chain A: 



### 4.2.15 Score per residue for model 15

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A: 



### 4.2.16 Score per residue for model 16

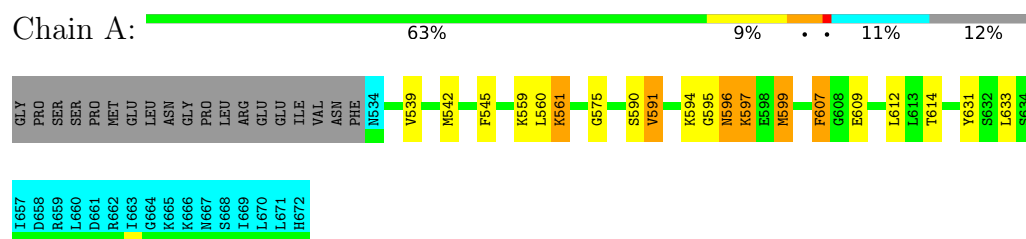
- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A: 



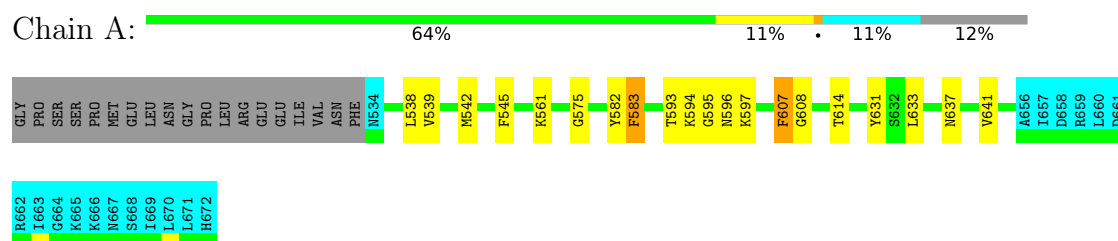
#### 4.2.17 Score per residue for model 17

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



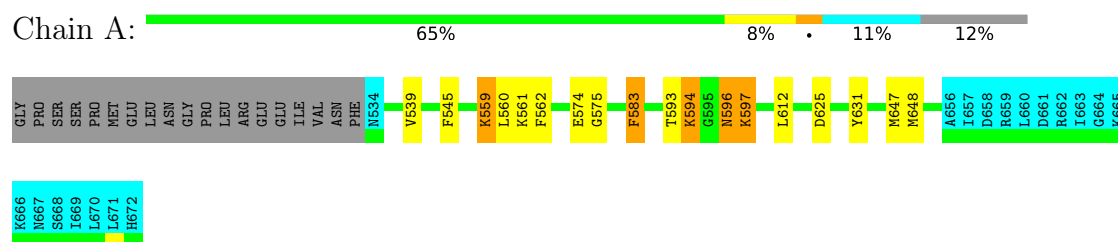
#### 4.2.18 Score per residue for model 18

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



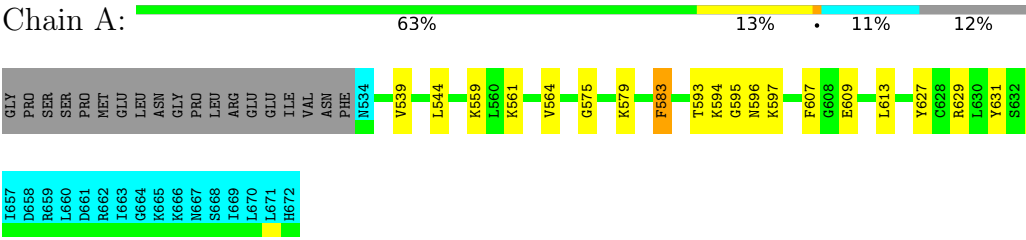
#### 4.2.19 Score per residue for model 19

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



4.2.20 Score per residue for model 20

- Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2



## 5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 2.1     |
| Amber         | refinement         | 12      |
| CANDID        | structure solution |         |
| CYANA         | refinement         |         |

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

|                                              |                |
|----------------------------------------------|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 1886           |
| Number of shifts mapped to atoms             | 1673           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 213            |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 87%            |

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 0.86±0.02    | 0±0/987 ( 0.0± 0.0%) | 1.50±0.04   | 4±2/1328 ( 0.3± 0.2%) |
| All | All   | 0.86         | 0/19740 ( 0.0%)      | 1.50        | 83/26560 ( 0.3%)      |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 3.5±1.6   |
| All | All   | 0         | 69        |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 583 | PHE  | CA-CB-CG   | 11.99 | 125.79      | 113.80   | 18     | 11    |
| 1   | A     | 596 | ASN  | CA-CB-CG   | 9.95  | 122.55      | 112.60   | 19     | 17    |
| 1   | A     | 638 | PHE  | CA-CB-CG   | 8.89  | 122.69      | 113.80   | 3      | 6     |
| 1   | A     | 607 | PHE  | CA-CB-CG   | 6.03  | 119.83      | 113.80   | 17     | 3     |
| 1   | A     | 622 | VAL  | N-CA-C     | 5.91  | 115.62      | 108.06   | 16     | 1     |
| 1   | A     | 571 | ILE  | CA-CB-CG1  | 5.83  | 120.32      | 110.40   | 14     | 2     |
| 1   | A     | 591 | VAL  | CG1-CB-CG2 | -5.73 | 98.19       | 110.80   | 17     | 14    |
| 1   | A     | 652 | PHE  | CA-CB-CG   | 5.59  | 119.39      | 113.80   | 2      | 1     |
| 1   | A     | 635 | VAL  | CG1-CB-CG2 | -5.59 | 98.51       | 110.80   | 5      | 3     |
| 1   | A     | 549 | ASP  | CA-C-N     | 5.40  | 125.07      | 119.56   | 1      | 1     |
| 1   | A     | 549 | ASP  | C-N-CA     | 5.40  | 125.07      | 119.56   | 1      | 1     |
| 1   | A     | 611 | CYS  | CA-C-N     | 5.38  | 128.02      | 120.28   | 6      | 1     |
| 1   | A     | 611 | CYS  | C-N-CA     | 5.38  | 128.02      | 120.28   | 6      | 1     |
| 1   | A     | 639 | ASN  | CA-CB-CG   | 5.36  | 117.96      | 112.60   | 3      | 1     |
| 1   | A     | 545 | PHE  | CA-CB-CG   | 5.32  | 119.12      | 113.80   | 7      | 5     |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
|     |       |     |      |            |       |             |          | Worst  | Total |
| 1   | A     | 609 | GLU  | CA-C-N     | 5.28  | 131.47      | 121.97   | 5      | 1     |
| 1   | A     | 609 | GLU  | C-N-CA     | 5.28  | 131.47      | 121.97   | 5      | 1     |
| 1   | A     | 594 | LYS  | N-CA-C     | 5.26  | 117.70      | 111.33   | 8      | 1     |
| 1   | A     | 559 | LYS  | CA-C-N     | 5.24  | 128.53      | 120.82   | 3      | 1     |
| 1   | A     | 559 | LYS  | C-N-CA     | 5.24  | 128.53      | 120.82   | 3      | 1     |
| 1   | A     | 576 | THR  | CA-C-N     | 5.23  | 128.43      | 120.95   | 3      | 1     |
| 1   | A     | 576 | THR  | C-N-CA     | 5.23  | 128.43      | 120.95   | 3      | 1     |
| 1   | A     | 560 | LEU  | CB-CA-C    | 5.22  | 119.15      | 109.54   | 7      | 1     |
| 1   | A     | 622 | VAL  | CA-CB-CG1  | 5.22  | 119.27      | 110.40   | 3      | 1     |
| 1   | A     | 559 | LYS  | CB-CA-C    | 5.13  | 119.27      | 110.85   | 19     | 1     |
| 1   | A     | 555 | ALA  | CA-C-N     | 5.13  | 127.67      | 120.28   | 3      | 1     |
| 1   | A     | 555 | ALA  | C-N-CA     | 5.13  | 127.67      | 120.28   | 3      | 1     |
| 1   | A     | 596 | ASN  | N-CA-C     | 5.05  | 116.87      | 109.24   | 19     | 1     |
| 1   | A     | 596 | ASN  | OD1-CG-ND2 | -5.05 | 117.55      | 122.60   | 8      | 1     |
| 1   | A     | 614 | THR  | N-CA-C     | 5.03  | 116.81      | 110.33   | 18     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 595 | GLY  | Peptide   | 16             |
| 1   | A     | 590 | SER  | Peptide   | 14             |
| 1   | A     | 599 | MET  | Peptide   | 11             |
| 1   | A     | 606 | TYR  | Sidechain | 4              |
| 1   | A     | 545 | PHE  | Sidechain | 4              |
| 1   | A     | 582 | TYR  | Sidechain | 2              |
| 1   | A     | 645 | TYR  | Sidechain | 2              |
| 1   | A     | 649 | ARG  | Sidechain | 2              |
| 1   | A     | 607 | PHE  | Peptide   | 2              |
| 1   | A     | 610 | ILE  | Peptide   | 2              |
| 1   | A     | 597 | LYS  | Peptide   | 2              |
| 1   | A     | 596 | ASN  | Peptide   | 1              |
| 1   | A     | 572 | ILE  | Peptide   | 1              |
| 1   | A     | 631 | TYR  | Sidechain | 1              |
| 1   | A     | 613 | LEU  | Peptide   | 1              |
| 1   | A     | 593 | THR  | Peptide   | 1              |
| 1   | A     | 608 | GLY  | Peptide   | 1              |
| 1   | A     | 592 | LEU  | Peptide   | 1              |
| 1   | A     | 629 | ARG  | Sidechain | 1              |

## 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 968   | 981      | 981      | 1±1     |
| All | All   | 19360 | 19620    | 19620    | 23      |

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 1.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:612:LEU:HD23 | 1:A:635:VAL:HG22 | 0.62     | 1.71        | 17     | 6     |
| 1:A:637:ASN:O    | 1:A:641:VAL:HG12 | 0.57     | 2.00        | 18     | 2     |
| 1:A:564:VAL:HG11 | 1:A:627:TYR:CE1  | 0.48     | 2.42        | 9      | 5     |
| 1:A:591:VAL:HG12 | 1:A:599:MET:C    | 0.48     | 2.33        | 17     | 2     |
| 1:A:613:LEU:HD13 | 1:A:613:LEU:H    | 0.45     | 1.72        | 8      | 1     |
| 1:A:596:ASN:CA   | 1:A:597:LYS:HE3  | 0.45     | 2.42        | 7      | 3     |
| 1:A:596:ASN:HA   | 1:A:597:LYS:HE3  | 0.43     | 1.88        | 10     | 1     |
| 1:A:591:VAL:HG12 | 1:A:599:MET:O    | 0.43     | 2.14        | 17     | 1     |
| 1:A:583:PHE:CE1  | 1:A:631:TYR:CE2  | 0.41     | 3.08        | 4      | 1     |
| 1:A:560:LEU:HD23 | 1:A:561:LYS:N    | 0.41     | 2.30        | 17     | 1     |

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-----------------|---------------|------------|------------|-------------|----|
| 1   | A     | 121/158 (77%)   | 115±1 (95±1%) | 4±1 (3±1%) | 2±1 (1±1%) | 13          | 61 |
| All | All   | 2420/3160 (77%) | 2307 (95%)    | 83 (3%)    | 30 (1%)    | 13          | 61 |

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 575 | GLY  | 15             |
| 1   | A     | 610 | ILE  | 5              |
| 1   | A     | 612 | LEU  | 4              |
| 1   | A     | 609 | GLU  | 2              |
| 1   | A     | 535 | CYS  | 1              |
| 1   | A     | 611 | CYS  | 1              |
| 1   | A     | 608 | GLY  | 1              |
| 1   | A     | 594 | LYS  | 1              |

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

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

| Mol | Chain | Analysed        | Rotameric    | Outliers     | Percentiles |    |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1   | A     | 106/139 (76%)   | 91±3 (86±3%) | 15±3 (14±3%) | 5           | 44 |
| All | All   | 2120/2780 (76%) | 1820 (86%)   | 300 (14%)    | 5           | 44 |

All 58 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     | 539 | VAL  | 20             |
| 1   | A     | 561 | LYS  | 20             |
| 1   | A     | 594 | LYS  | 20             |
| 1   | A     | 597 | LYS  | 18             |
| 1   | A     | 593 | THR  | 13             |
| 1   | A     | 562 | PHE  | 13             |
| 1   | A     | 635 | VAL  | 12             |
| 1   | A     | 601 | LEU  | 11             |
| 1   | A     | 559 | LYS  | 11             |
| 1   | A     | 631 | TYR  | 10             |
| 1   | A     | 607 | PHE  | 9              |
| 1   | A     | 648 | MET  | 9              |
| 1   | A     | 542 | MET  | 8              |
| 1   | A     | 583 | PHE  | 8              |
| 1   | A     | 600 | LYS  | 6              |
| 1   | A     | 642 | LEU  | 6              |
| 1   | A     | 547 | ASN  | 6              |
| 1   | A     | 613 | LEU  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 614 | THR  | 5              |
| 1   | A     | 633 | LEU  | 5              |
| 1   | A     | 622 | VAL  | 5              |
| 1   | A     | 574 | GLU  | 5              |
| 1   | A     | 582 | TYR  | 4              |
| 1   | A     | 538 | LEU  | 4              |
| 1   | A     | 537 | LYS  | 4              |
| 1   | A     | 625 | ASP  | 4              |
| 1   | A     | 573 | ARG  | 3              |
| 1   | A     | 627 | TYR  | 3              |
| 1   | A     | 544 | LEU  | 3              |
| 1   | A     | 609 | GLU  | 3              |
| 1   | A     | 592 | LEU  | 3              |
| 1   | A     | 649 | ARG  | 3              |
| 1   | A     | 560 | LEU  | 3              |
| 1   | A     | 596 | ASN  | 3              |
| 1   | A     | 643 | GLU  | 3              |
| 1   | A     | 585 | GLN  | 2              |
| 1   | A     | 606 | TYR  | 2              |
| 1   | A     | 612 | LEU  | 2              |
| 1   | A     | 591 | VAL  | 2              |
| 1   | A     | 579 | LYS  | 2              |
| 1   | A     | 603 | ASP  | 2              |
| 1   | A     | 586 | HIS  | 2              |
| 1   | A     | 650 | ARG  | 2              |
| 1   | A     | 623 | ARG  | 1              |
| 1   | A     | 638 | PHE  | 1              |
| 1   | A     | 536 | ARG  | 1              |
| 1   | A     | 590 | SER  | 1              |
| 1   | A     | 618 | ARG  | 1              |
| 1   | A     | 636 | ASP  | 1              |
| 1   | A     | 640 | GLU  | 1              |
| 1   | A     | 558 | THR  | 1              |
| 1   | A     | 617 | ARG  | 1              |
| 1   | A     | 598 | GLU  | 1              |
| 1   | A     | 580 | LYS  | 1              |
| 1   | A     | 641 | VAL  | 1              |
| 1   | A     | 629 | ARG  | 1              |
| 1   | A     | 634 | SER  | 1              |
| 1   | A     | 647 | MET  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|                                         |      |
|-----------------------------------------|------|
| Total number of shifts                  | 1886 |
| Number of shifts mapped to atoms        | 1673 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 213  |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 2    |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 213 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 516 | PRO  | HA   | 4.511      | 0.020       | 1         |
| 1       | A     | 516 | PRO  | HB2  | 2.303      | 0.020       | 2         |
| 1       | A     | 516 | PRO  | HB3  | 2.103      | 0.020       | 2         |
| 1       | A     | 516 | PRO  | HD2  | 3.484      | 0.020       | 2         |
| 1       | A     | 516 | PRO  | HD3  | 3.44       | 0.020       | 2         |
| 1       | A     | 516 | PRO  | HG2  | 1.879      | 0.020       | 2         |
| 1       | A     | 516 | PRO  | HG3  | 1.771      | 0.020       | 2         |
| 1       | A     | 516 | PRO  | CA   | 62.224     | 0.3         | 1         |
| 1       | A     | 516 | PRO  | CB   | 34.52      | 0.3         | 1         |
| 1       | A     | 516 | PRO  | CD   | 50.251     | 0.3         | 1         |
| 1       | A     | 516 | PRO  | CG   | 24.622     | 0.3         | 1         |
| 1       | A     | 517 | SER  | HA   | 4.416      | 0.020       | 1         |
| 1       | A     | 517 | SER  | HB2  | 3.8        | 0.020       | 1         |
| 1       | A     | 517 | SER  | HB3  | 3.8        | 0.020       | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 517 | SER  | C    | 174.078    | 0.3         | 1         |
| 1       | A     | 517 | SER  | CA   | 58.273     | 0.3         | 1         |
| 1       | A     | 517 | SER  | CB   | 63.721     | 0.3         | 1         |
| 1       | A     | 518 | SER  | H    | 8.221      | 0.020       | 1         |
| 1       | A     | 518 | SER  | HA   | 3.796      | 0.020       | 1         |
| 1       | A     | 518 | SER  | HB2  | 3.798      | 0.020       | 1         |
| 1       | A     | 518 | SER  | HB3  | 3.798      | 0.020       | 1         |
| 1       | A     | 518 | SER  | CA   | 56.265     | 0.3         | 1         |
| 1       | A     | 518 | SER  | CB   | 63.262     | 0.3         | 1         |
| 1       | A     | 518 | SER  | N    | 118.569    | 0.3         | 1         |
| 1       | A     | 519 | PRO  | HA   | 4.335      | 0.020       | 1         |
| 1       | A     | 519 | PRO  | HB2  | 2.24       | 0.020       | 2         |
| 1       | A     | 519 | PRO  | HB3  | 1.858      | 0.020       | 2         |
| 1       | A     | 519 | PRO  | HD2  | 3.747      | 0.020       | 2         |
| 1       | A     | 519 | PRO  | HD3  | 3.656      | 0.020       | 2         |
| 1       | A     | 519 | PRO  | HG2  | 1.947      | 0.020       | 1         |
| 1       | A     | 519 | PRO  | HG3  | 1.947      | 0.020       | 1         |
| 1       | A     | 519 | PRO  | C    | 177.009    | 0.3         | 1         |
| 1       | A     | 519 | PRO  | CA   | 63.448     | 0.3         | 1         |
| 1       | A     | 519 | PRO  | CB   | 31.854     | 0.3         | 1         |
| 1       | A     | 519 | PRO  | CD   | 50.595     | 0.3         | 1         |
| 1       | A     | 519 | PRO  | CG   | 27.245     | 0.3         | 1         |
| 1       | A     | 520 | MET  | H    | 8.258      | 0.020       | 1         |
| 1       | A     | 520 | MET  | HA   | 4.321      | 0.020       | 1         |
| 1       | A     | 520 | MET  | HB2  | 1.985      | 0.020       | 2         |
| 1       | A     | 520 | MET  | HB3  | 1.912      | 0.020       | 2         |
| 1       | A     | 520 | MET  | HG2  | 2.513      | 0.020       | 2         |
| 1       | A     | 520 | MET  | HG3  | 2.466      | 0.020       | 2         |
| 1       | A     | 520 | MET  | C    | 176.293    | 0.3         | 1         |
| 1       | A     | 520 | MET  | CA   | 55.805     | 0.3         | 1         |
| 1       | A     | 520 | MET  | CB   | 32.709     | 0.3         | 1         |
| 1       | A     | 520 | MET  | CG   | 31.878     | 0.3         | 1         |
| 1       | A     | 520 | MET  | N    | 119.429    | 0.3         | 1         |
| 1       | A     | 521 | GLU  | H    | 8.21       | 0.020       | 1         |
| 1       | A     | 521 | GLU  | HA   | 4.198      | 0.020       | 1         |
| 1       | A     | 521 | GLU  | HB2  | 1.944      | 0.020       | 2         |
| 1       | A     | 521 | GLU  | HB3  | 1.858      | 0.020       | 2         |
| 1       | A     | 521 | GLU  | HG2  | 2.152      | 0.020       | 1         |
| 1       | A     | 521 | GLU  | HG3  | 2.152      | 0.020       | 1         |
| 1       | A     | 521 | GLU  | C    | 176.319    | 0.3         | 1         |
| 1       | A     | 521 | GLU  | CA   | 56.479     | 0.3         | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 521 | GLU  | CB   | 30.1       | 0.3         | 1         |
| 1       | A     | 521 | GLU  | CG   | 36.13      | 0.3         | 1         |
| 1       | A     | 521 | GLU  | N    | 121.524    | 0.3         | 1         |
| 1       | A     | 522 | LEU  | H    | 8.112      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HA   | 4.253      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HB2  | 1.502      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HB3  | 1.502      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HD11 | 0.832      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HD12 | 0.832      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HD13 | 0.832      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HD21 | 0.772      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HD22 | 0.772      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HD23 | 0.772      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | HG   | 1.528      | 0.020       | 1         |
| 1       | A     | 522 | LEU  | C    | 176.887    | 0.3         | 1         |
| 1       | A     | 522 | LEU  | CA   | 55.161     | 0.3         | 1         |
| 1       | A     | 522 | LEU  | CB   | 42.16      | 0.3         | 1         |
| 1       | A     | 522 | LEU  | CD1  | 24.692     | 0.3         | 1         |
| 1       | A     | 522 | LEU  | CD2  | 23.423     | 0.3         | 1         |
| 1       | A     | 522 | LEU  | CG   | 26.779     | 0.3         | 1         |
| 1       | A     | 522 | LEU  | N    | 122.766    | 0.3         | 1         |
| 1       | A     | 523 | ASN  | H    | 8.286      | 0.020       | 1         |
| 1       | A     | 523 | ASN  | HA   | 4.691      | 0.020       | 1         |
| 1       | A     | 523 | ASN  | HB2  | 2.768      | 0.020       | 2         |
| 1       | A     | 523 | ASN  | HB3  | 2.664      | 0.020       | 2         |
| 1       | A     | 523 | ASN  | HD21 | 7.514      | 0.020       | 1         |
| 1       | A     | 523 | ASN  | HD22 | 6.845      | 0.020       | 1         |
| 1       | A     | 523 | ASN  | C    | 175.081    | 0.3         | 1         |
| 1       | A     | 523 | ASN  | CA   | 53.023     | 0.3         | 1         |
| 1       | A     | 523 | ASN  | CB   | 39.104     | 0.3         | 1         |
| 1       | A     | 523 | ASN  | CG   | 176.659    | 0.3         | 1         |
| 1       | A     | 523 | ASN  | N    | 118.606    | 0.3         | 1         |
| 1       | A     | 523 | ASN  | ND2  | 112.953    | 0.3         | 1         |
| 1       | A     | 524 | GLY  | H    | 8.061      | 0.020       | 1         |
| 1       | A     | 524 | GLY  | HA2  | 3.987      | 0.020       | 1         |
| 1       | A     | 524 | GLY  | HA3  | 3.987      | 0.020       | 1         |
| 1       | A     | 524 | GLY  | CA   | 44.931     | 0.3         | 1         |
| 1       | A     | 524 | GLY  | N    | 108.964    | 0.3         | 1         |
| 1       | A     | 525 | PRO  | HA   | 4.443      | 0.020       | 1         |
| 1       | A     | 525 | PRO  | HB2  | 2.243      | 0.020       | 2         |
| 1       | A     | 525 | PRO  | HB3  | 2.183      | 0.020       | 2         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 525 | PRO  | HD2  | 3.514      | 0.020       | 1         |
| 1       | A     | 525 | PRO  | HD3  | 3.514      | 0.020       | 1         |
| 1       | A     | 525 | PRO  | HG2  | 1.948      | 0.020       | 2         |
| 1       | A     | 525 | PRO  | HG3  | 1.899      | 0.020       | 2         |
| 1       | A     | 525 | PRO  | C    | 177.141    | 0.3         | 1         |
| 1       | A     | 525 | PRO  | CA   | 63.096     | 0.3         | 1         |
| 1       | A     | 525 | PRO  | CB   | 32.16      | 0.3         | 1         |
| 1       | A     | 525 | PRO  | CD   | 49.638     | 0.3         | 1         |
| 1       | A     | 525 | PRO  | CG   | 26.909     | 0.3         | 1         |
| 1       | A     | 526 | LEU  | H    | 8.203      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | HA   | 4.247      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | HB2  | 1.557      | 0.020       | 2         |
| 1       | A     | 526 | LEU  | HB3  | 1.498      | 0.020       | 2         |
| 1       | A     | 526 | LEU  | HD11 | 0.832      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | HD12 | 0.832      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | HD13 | 0.832      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | HD21 | 0.775      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | HD22 | 0.775      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | HD23 | 0.775      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | HG   | 1.531      | 0.020       | 1         |
| 1       | A     | 526 | LEU  | C    | 177.423    | 0.3         | 1         |
| 1       | A     | 526 | LEU  | CA   | 55.254     | 0.3         | 1         |
| 1       | A     | 526 | LEU  | CB   | 42.118     | 0.3         | 1         |
| 1       | A     | 526 | LEU  | CD1  | 24.733     | 0.3         | 1         |
| 1       | A     | 526 | LEU  | CD2  | 23.518     | 0.3         | 1         |
| 1       | A     | 526 | LEU  | CG   | 26.818     | 0.3         | 1         |
| 1       | A     | 526 | LEU  | N    | 121.258    | 0.3         | 1         |
| 1       | A     | 527 | ARG  | H    | 8.116      | 0.020       | 1         |
| 1       | A     | 527 | ARG  | HA   | 4.165      | 0.020       | 1         |
| 1       | A     | 527 | ARG  | HB2  | 1.753      | 0.020       | 2         |
| 1       | A     | 527 | ARG  | HB3  | 1.713      | 0.020       | 2         |
| 1       | A     | 527 | ARG  | HD2  | 3.116      | 0.020       | 1         |
| 1       | A     | 527 | ARG  | HD3  | 3.116      | 0.020       | 1         |
| 1       | A     | 527 | ARG  | HG2  | 1.556      | 0.020       | 1         |
| 1       | A     | 527 | ARG  | HG3  | 1.556      | 0.020       | 1         |
| 1       | A     | 527 | ARG  | C    | 176.456    | 0.3         | 1         |
| 1       | A     | 527 | ARG  | CA   | 56.555     | 0.3         | 1         |
| 1       | A     | 527 | ARG  | CB   | 30.478     | 0.3         | 1         |
| 1       | A     | 527 | ARG  | CD   | 43.109     | 0.3         | 1         |
| 1       | A     | 527 | ARG  | CG   | 26.943     | 0.3         | 1         |
| 1       | A     | 527 | ARG  | N    | 121.455    | 0.3         | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 528 | GLU  | H    | 8.338      | 0.020       | 1         |
| 1       | A     | 528 | GLU  | HA   | 4.092      | 0.020       | 1         |
| 1       | A     | 528 | GLU  | HB2  | 1.943      | 0.020       | 2         |
| 1       | A     | 528 | GLU  | HB3  | 1.859      | 0.020       | 2         |
| 1       | A     | 528 | GLU  | HG2  | 2.154      | 0.020       | 1         |
| 1       | A     | 528 | GLU  | HG3  | 2.154      | 0.020       | 1         |
| 1       | A     | 528 | GLU  | C    | 176.574    | 0.3         | 1         |
| 1       | A     | 528 | GLU  | CA   | 57.209     | 0.3         | 1         |
| 1       | A     | 528 | GLU  | CB   | 29.972     | 0.3         | 1         |
| 1       | A     | 528 | GLU  | CG   | 36.194     | 0.3         | 1         |
| 1       | A     | 528 | GLU  | N    | 121.28     | 0.3         | 1         |
| 1       | A     | 529 | GLU  | H    | 8.366      | 0.020       | 1         |
| 1       | A     | 529 | GLU  | HA   | 4.097      | 0.020       | 1         |
| 1       | A     | 529 | GLU  | HB2  | 1.941      | 0.020       | 2         |
| 1       | A     | 529 | GLU  | HB3  | 1.866      | 0.020       | 2         |
| 1       | A     | 529 | GLU  | HG2  | 2.154      | 0.020       | 1         |
| 1       | A     | 529 | GLU  | HG3  | 2.154      | 0.020       | 1         |
| 1       | A     | 529 | GLU  | C    | 176.85     | 0.3         | 1         |
| 1       | A     | 529 | GLU  | CA   | 57.056     | 0.3         | 1         |
| 1       | A     | 529 | GLU  | CB   | 29.838     | 0.3         | 1         |
| 1       | A     | 529 | GLU  | CG   | 36.171     | 0.3         | 1         |
| 1       | A     | 529 | GLU  | N    | 120.988    | 0.3         | 1         |
| 1       | A     | 530 | ILE  | H    | 7.941      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | HA   | 4.004      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | HB   | 1.803      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | HD11 | 0.719      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | HD12 | 0.719      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | HD13 | 0.719      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | HG12 | 1.375      | 0.020       | 2         |
| 1       | A     | 530 | ILE  | HG13 | 1.093      | 0.020       | 2         |
| 1       | A     | 530 | ILE  | HG21 | 0.789      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | HG22 | 0.789      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | HG23 | 0.789      | 0.020       | 1         |
| 1       | A     | 530 | ILE  | C    | 176.611    | 0.3         | 1         |
| 1       | A     | 530 | ILE  | CA   | 61.653     | 0.3         | 1         |
| 1       | A     | 530 | ILE  | CB   | 38.119     | 0.3         | 1         |
| 1       | A     | 530 | ILE  | CD1  | 12.603     | 0.3         | 1         |
| 1       | A     | 530 | ILE  | CG1  | 27.436     | 0.3         | 1         |
| 1       | A     | 530 | ILE  | CG2  | 17.405     | 0.3         | 1         |
| 1       | A     | 530 | ILE  | N    | 121.269    | 0.3         | 1         |
| 1       | A     | 531 | VAL  | H    | 7.952      | 0.020       | 1         |

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| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 531 | VAL  | HA   | 3.862      | 0.020       | 1         |
| 1       | A     | 531 | VAL  | HB   | 1.92       | 0.020       | 1         |
| 1       | A     | 531 | VAL  | HG11 | 0.767      | 0.020       | 1         |
| 1       | A     | 531 | VAL  | HG12 | 0.767      | 0.020       | 1         |
| 1       | A     | 531 | VAL  | HG13 | 0.767      | 0.020       | 1         |
| 1       | A     | 531 | VAL  | HG21 | 0.767      | 0.020       | 1         |
| 1       | A     | 531 | VAL  | HG22 | 0.767      | 0.020       | 1         |
| 1       | A     | 531 | VAL  | HG23 | 0.767      | 0.020       | 1         |
| 1       | A     | 531 | VAL  | C    | 176.308    | 0.3         | 1         |
| 1       | A     | 531 | VAL  | CA   | 63.257     | 0.3         | 1         |
| 1       | A     | 531 | VAL  | CB   | 32.11      | 0.3         | 1         |
| 1       | A     | 531 | VAL  | CG1  | 20.932     | 0.3         | 1         |
| 1       | A     | 531 | VAL  | N    | 122.87     | 0.3         | 1         |
| 1       | A     | 532 | ASN  | H    | 8.267      | 0.020       | 1         |
| 1       | A     | 532 | ASN  | HA   | 4.502      | 0.020       | 1         |
| 1       | A     | 532 | ASN  | HB2  | 2.682      | 0.020       | 1         |
| 1       | A     | 532 | ASN  | HB3  | 2.682      | 0.020       | 1         |
| 1       | A     | 532 | ASN  | HD21 | 7.516      | 0.020       | 1         |
| 1       | A     | 532 | ASN  | HD22 | 6.786      | 0.020       | 1         |
| 1       | A     | 532 | ASN  | C    | 175.26     | 0.3         | 1         |
| 1       | A     | 532 | ASN  | CA   | 53.718     | 0.3         | 1         |
| 1       | A     | 532 | ASN  | CB   | 38.469     | 0.3         | 1         |
| 1       | A     | 532 | ASN  | N    | 120.311    | 0.3         | 1         |
| 1       | A     | 532 | ASN  | ND2  | 112.632    | 0.3         | 1         |
| 1       | A     | 533 | PHE  | H    | 8.055      | 0.020       | 1         |
| 1       | A     | 533 | PHE  | HA   | 4.289      | 0.020       | 1         |
| 1       | A     | 533 | PHE  | HB2  | 3.105      | 0.020       | 2         |
| 1       | A     | 533 | PHE  | HB3  | 2.973      | 0.020       | 2         |
| 1       | A     | 533 | PHE  | HD1  | 7.247      | 0.020       | 1         |
| 1       | A     | 533 | PHE  | HD2  | 7.247      | 0.020       | 1         |
| 1       | A     | 533 | PHE  | HE1  | 7.181      | 0.020       | 1         |
| 1       | A     | 533 | PHE  | HE2  | 7.181      | 0.020       | 1         |
| 1       | A     | 533 | PHE  | CA   | 59.097     | 0.3         | 1         |
| 1       | A     | 533 | PHE  | CB   | 39.05      | 0.3         | 1         |
| 1       | A     | 533 | PHE  | N    | 120.952    | 0.3         | 1         |

### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 152      | $0.07 \pm 0.20$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 142      | $0.12 \pm 0.11$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 131      | $0.15 \pm 0.19$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 139      | $0.49 \pm 0.43$                 | None needed ( $< 0.5$ ppm) |

### 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 87%, i.e. 1479 atoms were assigned a chemical shift out of a possible 1698. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone  | 576/605 (95%)   | 240/246 (98%) | 224/242 (93%)   | 112/117 (96%)   |
| Sidechain | 839/952 (88%)   | 570/620 (92%) | 261/290 (90%)   | 8/42 (19%)      |
| Aromatic  | 64/141 (45%)    | 63/68 (93%)   | 1/72 (1%)       | 0/1 (0%)        |
| Overall   | 1479/1698 (87%) | 873/934 (93%) | 486/604 (80%)   | 120/160 (75%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1673 atoms were assigned a chemical shift out of a possible 1968. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 645/696 (93%)   | 269/283 (95%)  | 251/278 (90%)   | 125/135 (93%)   |
| Sidechain | 963/1124 (86%)  | 655/731 (90%)  | 300/341 (88%)   | 8/52 (15%)      |
| Aromatic  | 65/148 (44%)    | 64/72 (89%)    | 1/74 (1%)       | 0/2 (0%)        |
| Overall   | 1673/1968 (85%) | 988/1086 (91%) | 552/693 (80%)   | 133/189 (70%)   |

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

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

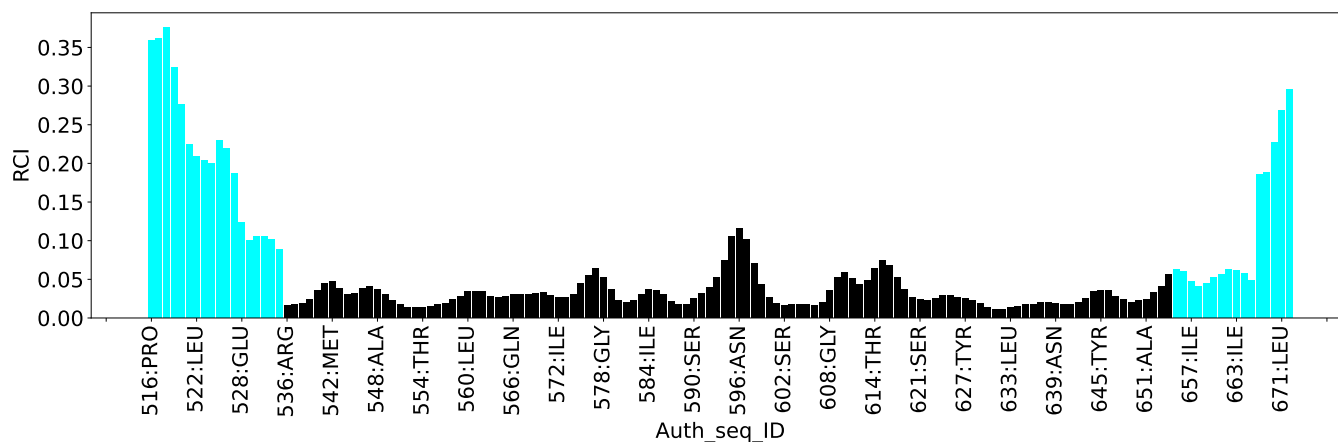
| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 582 | TYR  | HB3  | 0.61       | 0.93 – 4.76         | -5.8    |
| 1       | A     | 571 | ILE  | HG13 | -1.10      | -0.82 – 3.23        | -5.7    |

### 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                                | 1687  |
| Intra-residue ( $ i-j =0$ )                              | 406   |
| Sequential ( $ i-j =1$ )                                 | 534   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 262   |
| Long range ( $ i-j \geq 5$ )                             | 449   |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 36    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 198   |
| Number of unmapped restraints                            | 103   |
| Number of restraints per residue                         | 11.9  |
| Number of long range restraints per residue <sup>1</sup> | 3.1   |

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

### 8.2 Residual restraint violations

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

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

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

| Bins (Å)         | Average number of violations per model | Max (Å) |
|------------------|----------------------------------------|---------|
| 0.1-0.2 (Small)  | 5.5                                    | 0.2     |
| 0.2-0.5 (Medium) | 6.8                                    | 0.5     |
| >0.5 (Large)     | 9.7                                    | 2.12    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|----------------------------------------|---------|
| 1.0-10.0 (Small)   | 14.2                                   | 8.89    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

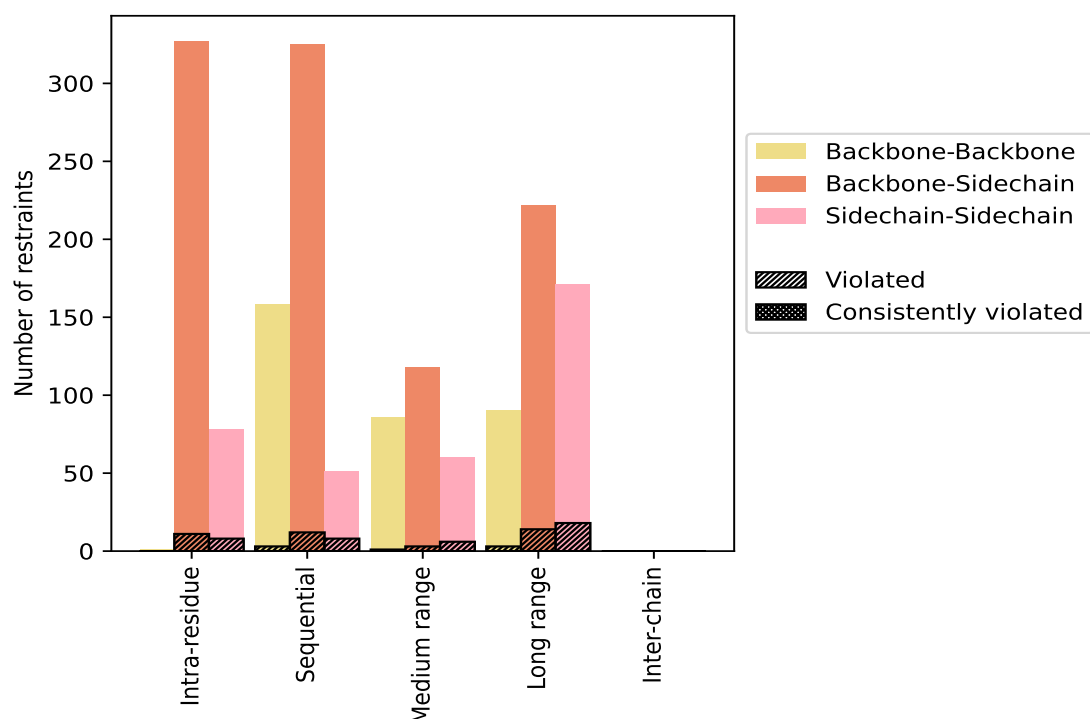
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>406</b>  | <b>24.1</b>    | <b>19</b>             | <b>4.7</b>     | <b>1.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 1           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 327         | 19.4           | 11                    | 3.4            | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 78          | 4.6            | 8                     | 10.3           | 0.5            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>534</b>  | <b>31.7</b>    | <b>23</b>             | <b>4.3</b>     | <b>1.4</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 158         | 9.4            | 3                     | 1.9            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 325         | 19.3           | 12                    | 3.7            | 0.7            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 51          | 3.0            | 8                     | 15.7           | 0.5            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>262</b>  | <b>15.5</b>    | <b>10</b>             | <b>3.8</b>     | <b>0.6</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 86          | 5.1            | 1                     | 1.2            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 116         | 6.9            | 3                     | 2.6            | 0.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 60          | 3.6            | 6                     | 10.0           | 0.4            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>449</b>  | <b>26.6</b>    | <b>35</b>             | <b>7.8</b>     | <b>2.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 90          | 5.3            | 3                     | 3.3            | 0.2            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 188         | 11.1           | 14                    | 7.4            | 0.8            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 171         | 10.1           | 18                    | 10.5           | 1.1            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0           | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>36</b>   | <b>2.1</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>1687</b> | <b>100.0</b>   | <b>87</b>             | <b>5.2</b>     | <b>5.2</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 335         | 19.9           | 7                     | 2.1            | 0.4            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 992         | 58.8           | 40                    | 4.0            | 2.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 360         | 21.3           | 40                    | 11.1           | 2.4            | 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        | 5                    | 6               | 7               | 9               | 0               | 27    | 0.45     | 1.65    | 0.44                | 0.2        |
| 2        | 1                    | 3               | 6               | 10              | 0               | 20    | 0.6      | 1.35    | 0.4                 | 0.56       |
| 3        | 3                    | 6               | 4               | 9               | 0               | 22    | 0.58     | 2.09    | 0.56                | 0.36       |
| 4        | 3                    | 7               | 6               | 10              | 0               | 26    | 0.64     | 1.82    | 0.52                | 0.55       |
| 5        | 2                    | 7               | 6               | 10              | 0               | 25    | 0.67     | 1.73    | 0.5                 | 0.45       |
| 6        | 3                    | 3               | 7               | 13              | 0               | 26    | 0.55     | 2.08    | 0.5                 | 0.42       |
| 7        | 7                    | 3               | 6               | 10              | 0               | 26    | 0.51     | 2.12    | 0.49                | 0.38       |
| 8        | 3                    | 6               | 3               | 10              | 0               | 22    | 0.55     | 1.5     | 0.36                | 0.49       |
| 9        | 2                    | 4               | 5               | 19              | 0               | 30    | 0.44     | 1.53    | 0.35                | 0.33       |
| 10       | 0                    | 5               | 5               | 7               | 0               | 17    | 0.57     | 1.29    | 0.38                | 0.55       |

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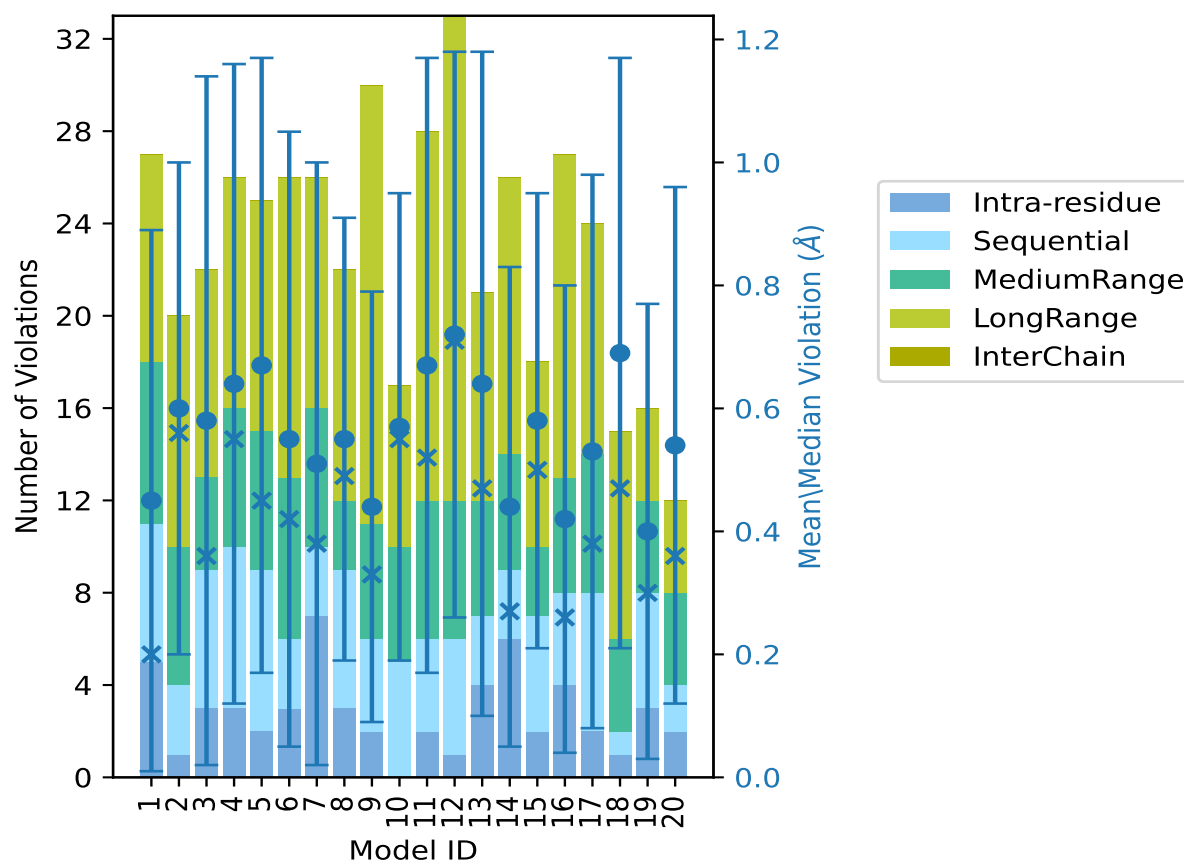
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 2                    | 4               | 6               | 16              | 0               | 28    | 0.67     | 1.82    | 0.5                 | 0.52       |
| 12       | 1                    | 5               | 6               | 21              | 0               | 33    | 0.72     | 1.75    | 0.46                | 0.71       |
| 13       | 4                    | 3               | 5               | 9               | 0               | 21    | 0.64     | 2.11    | 0.54                | 0.47       |
| 14       | 6                    | 3               | 5               | 12              | 0               | 26    | 0.44     | 1.52    | 0.39                | 0.27       |
| 15       | 2                    | 5               | 3               | 8               | 0               | 18    | 0.58     | 1.52    | 0.37                | 0.5        |
| 16       | 4                    | 4               | 5               | 14              | 0               | 27    | 0.42     | 1.45    | 0.38                | 0.26       |
| 17       | 2                    | 6               | 6               | 10              | 0               | 24    | 0.53     | 1.84    | 0.45                | 0.38       |
| 18       | 1                    | 1               | 4               | 9               | 0               | 15    | 0.69     | 1.8     | 0.48                | 0.47       |
| 19       | 3                    | 5               | 4               | 4               | 0               | 16    | 0.4      | 1.42    | 0.37                | 0.3        |
| 20       | 2                    | 2               | 4               | 4               | 0               | 12    | 0.54     | 1.51    | 0.42                | 0.36       |

<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

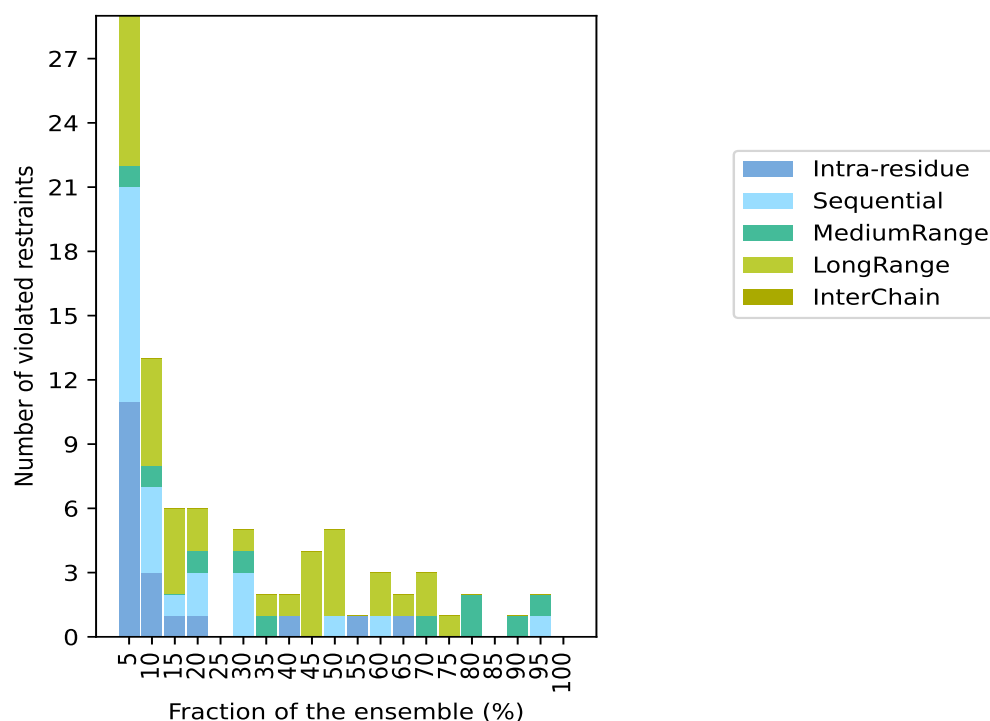
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1564(IR:387, SQ:511, MR:252, LR:414, IC:0) restraints are 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>       | %     |
| 11                            | 10              | 1               | 7               | 0               | 29    | 1                        | 5.0   |
| 3                             | 4               | 1               | 5               | 0               | 13    | 2                        | 10.0  |
| 1                             | 1               | 0               | 4               | 0               | 6     | 3                        | 15.0  |
| 1                             | 2               | 1               | 2               | 0               | 6     | 4                        | 20.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 5                        | 25.0  |
| 0                             | 3               | 1               | 1               | 0               | 5     | 6                        | 30.0  |
| 0                             | 0               | 1               | 1               | 0               | 2     | 7                        | 35.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 8                        | 40.0  |
| 0                             | 0               | 0               | 4               | 0               | 4     | 9                        | 45.0  |
| 0                             | 1               | 0               | 4               | 0               | 5     | 10                       | 50.0  |
| 1                             | 0               | 0               | 0               | 0               | 1     | 11                       | 55.0  |
| 0                             | 1               | 0               | 2               | 0               | 3     | 12                       | 60.0  |
| 1                             | 0               | 0               | 1               | 0               | 2     | 13                       | 65.0  |
| 0                             | 0               | 1               | 2               | 0               | 3     | 14                       | 70.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 15                       | 75.0  |
| 0                             | 0               | 2               | 0               | 0               | 2     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 0               | 1               | 0               | 0               | 1     | 18                       | 90.0  |
| 0                             | 1               | 1               | 0               | 0               | 2     | 19                       | 95.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 20                       | 100.0 |

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

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

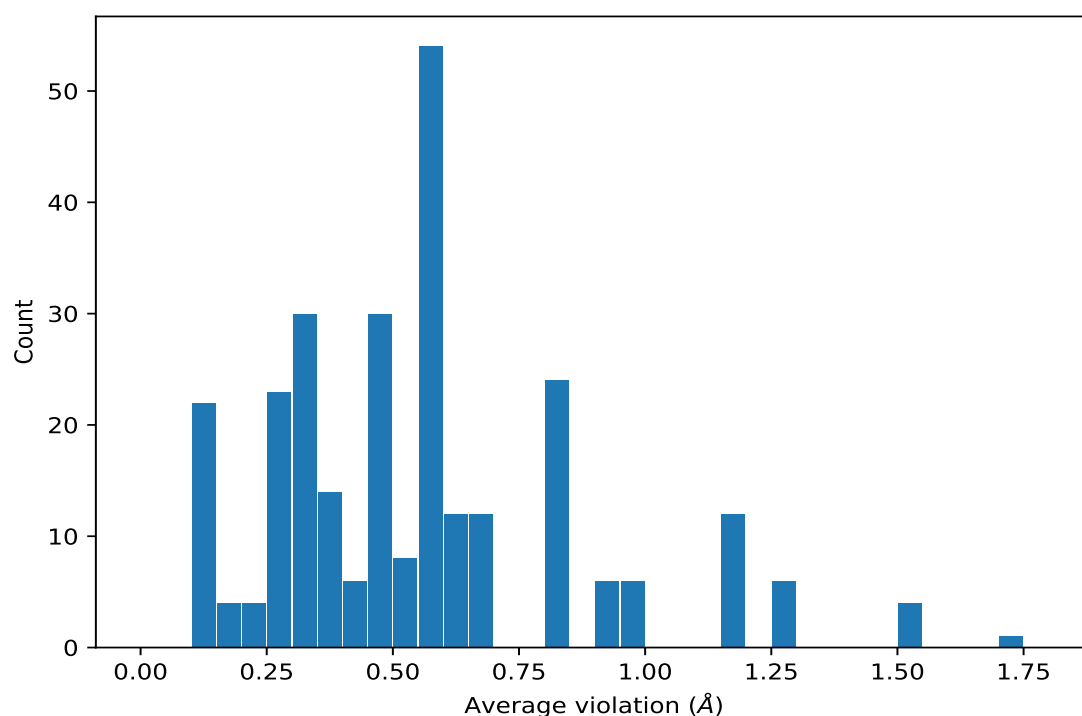
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 19                  | 0.98     | 0.45                | 0.95       |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 19                  | 0.98     | 0.45                | 0.95       |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 19                  | 0.98     | 0.45                | 0.95       |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 19                  | 0.98     | 0.45                | 0.95       |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 19                  | 0.98     | 0.45                | 0.95       |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 19                  | 0.98     | 0.45                | 0.95       |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 19                  | 0.67     | 0.22                | 0.72       |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 19                  | 0.67     | 0.22                | 0.72       |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 19                  | 0.67     | 0.22                | 0.72       |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 19                  | 0.67     | 0.22                | 0.72       |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 19                  | 0.67     | 0.22                | 0.72       |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 19                  | 0.67     | 0.22                | 0.72       |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 18                  | 1.18     | 0.54                | 1.38       |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 18                  | 1.18     | 0.54                | 1.38       |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 18                  | 1.18     | 0.54                | 1.38       |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 18                  | 1.18     | 0.54                | 1.38       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 18                  | 1.18     | 0.54                | 1.38       |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 18                  | 1.18     | 0.54                | 1.38       |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG21 | 16                  | 1.17     | 0.52                | 1.28       |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG22 | 16                  | 1.17     | 0.52                | 1.28       |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG23 | 16                  | 1.17     | 0.52                | 1.28       |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG21 | 16                  | 1.17     | 0.52                | 1.28       |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG22 | 16                  | 1.17     | 0.52                | 1.28       |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG23 | 16                  | 1.17     | 0.52                | 1.28       |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 16                  | 0.85     | 0.37                | 0.91       |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 16                  | 0.85     | 0.37                | 0.91       |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 16                  | 0.85     | 0.37                | 0.91       |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 16                  | 0.85     | 0.37                | 0.91       |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 16                  | 0.85     | 0.37                | 0.91       |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 16                  | 0.85     | 0.37                | 0.91       |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 15                  | 0.67     | 0.14                | 0.71       |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 15                  | 0.67     | 0.14                | 0.71       |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 15                  | 0.67     | 0.14                | 0.71       |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 15                  | 0.67     | 0.14                | 0.71       |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 15                  | 0.67     | 0.14                | 0.71       |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 15                  | 0.67     | 0.14                | 0.71       |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 14                  | 1.26     | 0.32                | 1.37       |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 14                  | 1.26     | 0.32                | 1.37       |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 14                  | 1.26     | 0.32                | 1.37       |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 14                  | 1.26     | 0.32                | 1.37       |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 14                  | 1.26     | 0.32                | 1.37       |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 14                  | 1.26     | 0.32                | 1.37       |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 14                  | 0.16     | 0.01                | 0.16       |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 14                  | 0.16     | 0.01                | 0.16       |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 14                  | 0.16     | 0.01                | 0.16       |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 14                  | 0.14     | 0.02                | 0.14       |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 13                  | 0.62     | 0.37                | 0.53       |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 13                  | 0.62     | 0.37                | 0.53       |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 13                  | 0.62     | 0.37                | 0.53       |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 13                  | 0.62     | 0.37                | 0.53       |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 13                  | 0.62     | 0.37                | 0.53       |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 13                  | 0.62     | 0.37                | 0.53       |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 13                  | 0.38     | 0.13                | 0.42       |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 13                  | 0.38     | 0.13                | 0.42       |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 13                  | 0.38     | 0.13                | 0.42       |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 13                  | 0.38     | 0.13                | 0.42       |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD2  | 12                  | 1.53     | 0.47                | 1.38       |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD3  | 12                  | 1.53     | 0.47                | 1.38       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD2  | 12                  | 1.53     | 0.47                | 1.38       |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD3  | 12                  | 1.53     | 0.47                | 1.38       |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 12                  | 0.82     | 0.15                | 0.8        |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 12                  | 0.82     | 0.15                | 0.8        |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 12                  | 0.82     | 0.15                | 0.8        |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 12                  | 0.82     | 0.15                | 0.8        |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 12                  | 0.82     | 0.15                | 0.8        |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 12                  | 0.82     | 0.15                | 0.8        |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 12                  | 0.55     | 0.26                | 0.5        |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 12                  | 0.55     | 0.26                | 0.5        |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 12                  | 0.55     | 0.26                | 0.5        |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 12                  | 0.55     | 0.26                | 0.5        |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 12                  | 0.55     | 0.26                | 0.5        |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 12                  | 0.55     | 0.26                | 0.5        |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 11                  | 0.34     | 0.08                | 0.32       |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 11                  | 0.34     | 0.08                | 0.32       |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 11                  | 0.34     | 0.08                | 0.32       |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 11                  | 0.34     | 0.08                | 0.32       |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 11                  | 0.34     | 0.08                | 0.32       |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 11                  | 0.34     | 0.08                | 0.32       |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD11 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD12 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD13 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD21 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD22 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD23 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD11 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 10                  | 0.8      | 0.41                | 0.67       |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 10                  | 0.56     | 0.27                | 0.54       |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 10                  | 0.56     | 0.27                | 0.54       |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 10                  | 0.56     | 0.27                | 0.54       |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 10                  | 0.56     | 0.27                | 0.54       |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 10                  | 0.56     | 0.27                | 0.54       |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 10                  | 0.56     | 0.27                | 0.54       |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 10                  | 0.45     | 0.18                | 0.5        |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 10                  | 0.45     | 0.18                | 0.5        |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 10                  | 0.45     | 0.18                | 0.5        |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 10                  | 0.45     | 0.18                | 0.5        |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 10                  | 0.45     | 0.18                | 0.5        |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 10                  | 0.45     | 0.18                | 0.5        |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 10                  | 0.3      | 0.15                | 0.28       |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 10                  | 0.3      | 0.15                | 0.28       |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 10                  | 0.3      | 0.15                | 0.28       |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 10                  | 0.3      | 0.15                | 0.28       |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 10                  | 0.3      | 0.15                | 0.28       |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 10                  | 0.3      | 0.15                | 0.28       |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 10                  | 0.13     | 0.02                | 0.12       |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 10                  | 0.13     | 0.02                | 0.12       |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 10                  | 0.13     | 0.02                | 0.12       |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 9                   | 0.6      | 0.35                | 0.73       |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 9                   | 0.6      | 0.35                | 0.73       |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 9                   | 0.6      | 0.35                | 0.73       |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 9                   | 0.6      | 0.35                | 0.73       |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 9                   | 0.6      | 0.35                | 0.73       |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 9                   | 0.6      | 0.35                | 0.73       |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3  | 9                   | 0.49     | 0.26                | 0.39       |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1  | 9                   | 0.41     | 0.16                | 0.41       |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2  | 9                   | 0.41     | 0.16                | 0.41       |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1  | 9                   | 0.41     | 0.16                | 0.41       |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2  | 9                   | 0.41     | 0.16                | 0.41       |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1  | 9                   | 0.41     | 0.16                | 0.41       |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2  | 9                   | 0.41     | 0.16                | 0.41       |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 9                   | 0.3      | 0.08                | 0.25       |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 9                   | 0.3      | 0.08                | 0.25       |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 9                   | 0.3      | 0.08                | 0.25       |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 9                   | 0.3      | 0.08                | 0.25       |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 9                   | 0.3      | 0.08                | 0.25       |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 9                   | 0.3      | 0.08                | 0.25       |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 8                   | 0.45     | 0.17                | 0.47       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 8                   | 0.45     | 0.17                | 0.47       |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 8                   | 0.45     | 0.17                | 0.47       |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 8                   | 0.45     | 0.17                | 0.47       |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 8                   | 0.45     | 0.17                | 0.47       |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 8                   | 0.45     | 0.17                | 0.47       |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 8                   | 0.37     | 0.11                | 0.36       |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 8                   | 0.37     | 0.11                | 0.36       |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 8                   | 0.37     | 0.11                | 0.36       |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 8                   | 0.37     | 0.11                | 0.36       |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD1  | 7                   | 0.29     | 0.12                | 0.24       |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD2  | 7                   | 0.29     | 0.12                | 0.24       |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD1  | 7                   | 0.29     | 0.12                | 0.24       |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD2  | 7                   | 0.29     | 0.12                | 0.24       |
| (1,1264) | 1:626:A:THR:H    | 1:628:A:CYS:HB2  | 7                   | 0.14     | 0.01                | 0.14       |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA2  | 6                   | 0.51     | 0.08                | 0.49       |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA3  | 6                   | 0.51     | 0.08                | 0.49       |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA2  | 6                   | 0.51     | 0.08                | 0.49       |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA3  | 6                   | 0.51     | 0.08                | 0.49       |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA2  | 6                   | 0.51     | 0.2                 | 0.5        |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA3  | 6                   | 0.51     | 0.2                 | 0.5        |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA2  | 6                   | 0.51     | 0.2                 | 0.5        |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA3  | 6                   | 0.51     | 0.2                 | 0.5        |
| (1,137)  | 1:538:A:LEU:HD11 | 1:584:A:ILE:H    | 6                   | 0.47     | 0.23                | 0.38       |
| (1,137)  | 1:538:A:LEU:HD12 | 1:584:A:ILE:H    | 6                   | 0.47     | 0.23                | 0.38       |
| (1,137)  | 1:538:A:LEU:HD13 | 1:584:A:ILE:H    | 6                   | 0.47     | 0.23                | 0.38       |
| (1,137)  | 1:538:A:LEU:HD21 | 1:584:A:ILE:H    | 6                   | 0.47     | 0.23                | 0.38       |
| (1,137)  | 1:538:A:LEU:HD22 | 1:584:A:ILE:H    | 6                   | 0.47     | 0.23                | 0.38       |
| (1,137)  | 1:538:A:LEU:HD23 | 1:584:A:ILE:H    | 6                   | 0.47     | 0.23                | 0.38       |
| (1,1327) | 1:635:A:VAL:HG21 | 1:636:A:ASP:HA   | 6                   | 0.15     | 0.01                | 0.15       |
| (1,1327) | 1:635:A:VAL:HG22 | 1:636:A:ASP:HA   | 6                   | 0.15     | 0.01                | 0.15       |
| (1,1327) | 1:635:A:VAL:HG23 | 1:636:A:ASP:HA   | 6                   | 0.15     | 0.01                | 0.15       |
| (1,1015) | 1:591:A:VAL:HG11 | 1:593:A:THR:H    | 6                   | 0.12     | 0.02                | 0.12       |
| (1,1015) | 1:591:A:VAL:HG12 | 1:593:A:THR:H    | 6                   | 0.12     | 0.02                | 0.12       |
| (1,1015) | 1:591:A:VAL:HG13 | 1:593:A:THR:H    | 6                   | 0.12     | 0.02                | 0.12       |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB2  | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB3  | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB2  | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB3  | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB2  | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB3  | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB2  | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB3  | 4                   | 0.58     | 0.28                | 0.55       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB2 | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB3 | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB2 | 4                   | 0.58     | 0.28                | 0.55       |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB3 | 4                   | 0.58     | 0.28                | 0.55       |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD1 | 4                   | 0.55     | 0.35                | 0.43       |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD2 | 4                   | 0.55     | 0.35                | 0.43       |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD1 | 4                   | 0.55     | 0.35                | 0.43       |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD2 | 4                   | 0.55     | 0.35                | 0.43       |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD1 | 4                   | 0.55     | 0.35                | 0.43       |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD2 | 4                   | 0.55     | 0.35                | 0.43       |
| (1,932)  | 1:588:A:VAL:HG11 | 1:602:A:SER:HB3 | 4                   | 0.32     | 0.04                | 0.31       |
| (1,932)  | 1:588:A:VAL:HG12 | 1:602:A:SER:HB3 | 4                   | 0.32     | 0.04                | 0.31       |
| (1,932)  | 1:588:A:VAL:HG13 | 1:602:A:SER:HB3 | 4                   | 0.32     | 0.04                | 0.31       |
| (1,932)  | 1:588:A:VAL:HG21 | 1:602:A:SER:HB3 | 4                   | 0.32     | 0.04                | 0.31       |
| (1,932)  | 1:588:A:VAL:HG22 | 1:602:A:SER:HB3 | 4                   | 0.32     | 0.04                | 0.31       |
| (1,932)  | 1:588:A:VAL:HG23 | 1:602:A:SER:HB3 | 4                   | 0.32     | 0.04                | 0.31       |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG2 | 4                   | 0.3      | 0.2                 | 0.22       |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG3 | 4                   | 0.3      | 0.2                 | 0.22       |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG2 | 4                   | 0.3      | 0.2                 | 0.22       |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG3 | 4                   | 0.3      | 0.2                 | 0.22       |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG2 | 4                   | 0.3      | 0.2                 | 0.22       |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG3 | 4                   | 0.3      | 0.2                 | 0.22       |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD2 | 4                   | 0.2      | 0.05                | 0.2        |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD3 | 4                   | 0.2      | 0.05                | 0.2        |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD2 | 4                   | 0.2      | 0.05                | 0.2        |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD3 | 4                   | 0.2      | 0.05                | 0.2        |
| (1,1127) | 1:600:A:LYS:HD3  | 1:601:A:LEU:H   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,142)  | 1:538:A:LEU:HD11 | 1:586:A:HIS:H   | 3                   | 0.62     | 0.31                | 0.55       |
| (1,142)  | 1:538:A:LEU:HD12 | 1:586:A:HIS:H   | 3                   | 0.62     | 0.31                | 0.55       |
| (1,142)  | 1:538:A:LEU:HD13 | 1:586:A:HIS:H   | 3                   | 0.62     | 0.31                | 0.55       |
| (1,142)  | 1:538:A:LEU:HD21 | 1:586:A:HIS:H   | 3                   | 0.62     | 0.31                | 0.55       |
| (1,142)  | 1:538:A:LEU:HD22 | 1:586:A:HIS:H   | 3                   | 0.62     | 0.31                | 0.55       |
| (1,142)  | 1:538:A:LEU:HD23 | 1:586:A:HIS:H   | 3                   | 0.62     | 0.31                | 0.55       |
| (1,138)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:H   | 3                   | 0.58     | 0.21                | 0.49       |
| (1,138)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:H   | 3                   | 0.58     | 0.21                | 0.49       |
| (1,138)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:H   | 3                   | 0.58     | 0.21                | 0.49       |
| (1,138)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:H   | 3                   | 0.58     | 0.21                | 0.49       |
| (1,138)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:H   | 3                   | 0.58     | 0.21                | 0.49       |
| (1,138)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:H   | 3                   | 0.58     | 0.21                | 0.49       |
| (1,139)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HA  | 3                   | 0.57     | 0.33                | 0.56       |
| (1,139)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HA  | 3                   | 0.57     | 0.33                | 0.56       |
| (1,139)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HA  | 3                   | 0.57     | 0.33                | 0.56       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,139)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HA   | 3                   | 0.57     | 0.33                | 0.56       |
| (1,139)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HA   | 3                   | 0.57     | 0.33                | 0.56       |
| (1,139)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HA   | 3                   | 0.57     | 0.33                | 0.56       |
| (1,1043) | 1:592:A:LEU:HD11 | 1:599:A:MET:H    | 3                   | 0.39     | 0.3                 | 0.24       |
| (1,1043) | 1:592:A:LEU:HD12 | 1:599:A:MET:H    | 3                   | 0.39     | 0.3                 | 0.24       |
| (1,1043) | 1:592:A:LEU:HD13 | 1:599:A:MET:H    | 3                   | 0.39     | 0.3                 | 0.24       |
| (1,1043) | 1:592:A:LEU:HD21 | 1:599:A:MET:H    | 3                   | 0.39     | 0.3                 | 0.24       |
| (1,1043) | 1:592:A:LEU:HD22 | 1:599:A:MET:H    | 3                   | 0.39     | 0.3                 | 0.24       |
| (1,1043) | 1:592:A:LEU:HD23 | 1:599:A:MET:H    | 3                   | 0.39     | 0.3                 | 0.24       |
| (1,1427) | 1:643:A:GLU:H    | 1:643:A:GLU:HB2  | 3                   | 0.13     | 0.01                | 0.14       |
| (1,1074) | 1:595:A:GLY:HA2  | 1:596:A:ASN:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1074) | 1:595:A:GLY:HA3  | 1:596:A:ASN:HB3  | 3                   | 0.11     | 0.0                 | 0.11       |
| (1,1336) | 1:636:A:ASP:HB2  | 1:637:A:ASN:HD22 | 2                   | 1.74     | 0.01                | 1.74       |
| (1,1476) | 1:647:A:MET:HE1  | 1:648:A:MET:HG2  | 2                   | 0.94     | 0.05                | 0.94       |
| (1,1476) | 1:647:A:MET:HE1  | 1:648:A:MET:HG3  | 2                   | 0.94     | 0.05                | 0.94       |
| (1,1476) | 1:647:A:MET:HE2  | 1:648:A:MET:HG2  | 2                   | 0.94     | 0.05                | 0.94       |
| (1,1476) | 1:647:A:MET:HE2  | 1:648:A:MET:HG3  | 2                   | 0.94     | 0.05                | 0.94       |
| (1,1476) | 1:647:A:MET:HE3  | 1:648:A:MET:HG2  | 2                   | 0.94     | 0.05                | 0.94       |
| (1,1476) | 1:647:A:MET:HE3  | 1:648:A:MET:HG3  | 2                   | 0.94     | 0.05                | 0.94       |
| (1,211)  | 1:542:A:MET:HE1  | 1:606:A:TYR:HD1  | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,211)  | 1:542:A:MET:HE1  | 1:606:A:TYR:HD2  | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,211)  | 1:542:A:MET:HE2  | 1:606:A:TYR:HD1  | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,211)  | 1:542:A:MET:HE2  | 1:606:A:TYR:HD2  | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,211)  | 1:542:A:MET:HE3  | 1:606:A:TYR:HD1  | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,211)  | 1:542:A:MET:HE3  | 1:606:A:TYR:HD2  | 2                   | 0.56     | 0.2                 | 0.56       |
| (1,968)  | 1:589:A:VAL:HG21 | 1:607:A:PHE:HD1  | 2                   | 0.33     | 0.01                | 0.33       |
| (1,968)  | 1:589:A:VAL:HG21 | 1:607:A:PHE:HD2  | 2                   | 0.33     | 0.01                | 0.33       |
| (1,968)  | 1:589:A:VAL:HG22 | 1:607:A:PHE:HD1  | 2                   | 0.33     | 0.01                | 0.33       |
| (1,968)  | 1:589:A:VAL:HG22 | 1:607:A:PHE:HD2  | 2                   | 0.33     | 0.01                | 0.33       |
| (1,968)  | 1:589:A:VAL:HG23 | 1:607:A:PHE:HD1  | 2                   | 0.33     | 0.01                | 0.33       |
| (1,968)  | 1:589:A:VAL:HG23 | 1:607:A:PHE:HD2  | 2                   | 0.33     | 0.01                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HB2  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HB3  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HB2  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HB3  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HB2  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HB3  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HB2  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HB3  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HB2  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HB3  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1042) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HB2  | 2                   | 0.33     | 0.13                | 0.33       |

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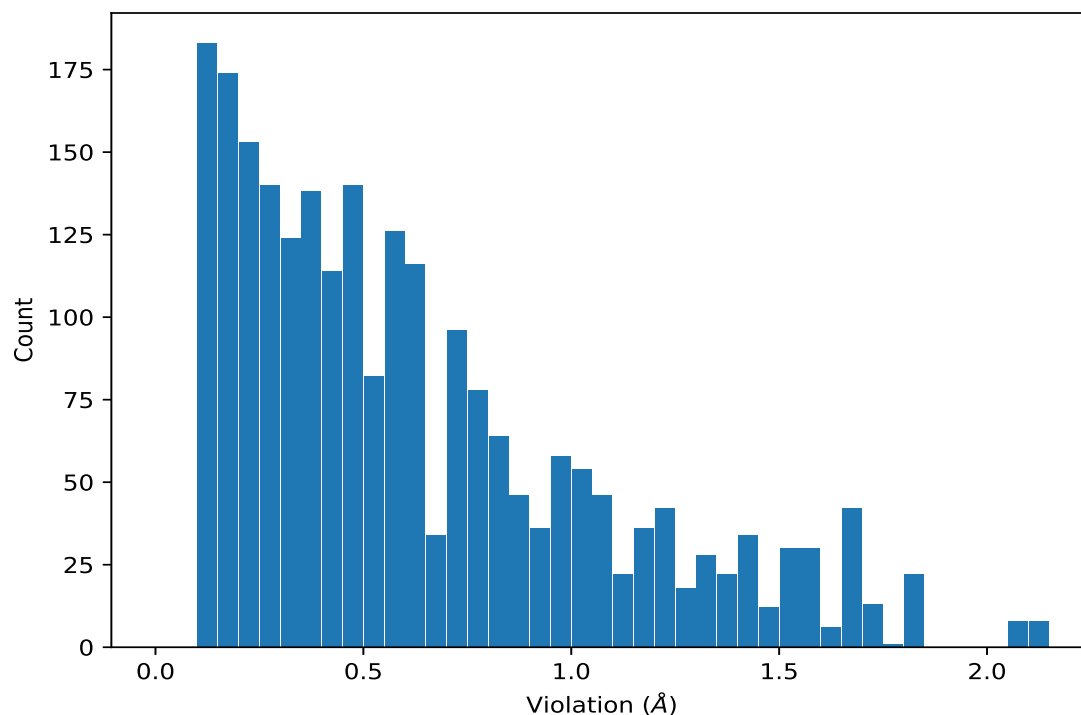
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1042) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HB3  | 2                   | 0.33     | 0.13                | 0.33       |
| (1,1612) | 1:663:A:ILE:HA   | 1:663:A:ILE:HG12 | 2                   | 0.26     | 0.01                | 0.26       |
| (1,1429) | 1:643:A:GLU:HB2  | 1:643:A:GLU:HG2  | 2                   | 0.16     | 0.04                | 0.16       |
| (1,1185) | 1:611:A:CYS:HA   | 1:614:A:THR:H    | 2                   | 0.14     | 0.04                | 0.14       |
| (1,696)  | 1:574:A:GLU:HA   | 1:579:A:LYS:HD2  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,696)  | 1:574:A:GLU:HA   | 1:579:A:LYS:HD3  | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1588) | 1:659:A:ARG:H    | 1:659:A:ARG:HB2  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,257)  | 1:546:A:ALA:H    | 1:547:A:ASN:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,567)  | 1:566:A:GLN:HA   | 1:627:A:TYR:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,595)  | 1:568:A:GLY:H    | 1:569:A:ASP:HA   | 2                   | 0.1      | 0.0                 | 0.1        |

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

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

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

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



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

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

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD2  | 7        | 2.12          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD3  | 7        | 2.12          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD2  | 7        | 2.12          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD3  | 7        | 2.12          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD2  | 13       | 2.11          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD3  | 13       | 2.11          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD2  | 13       | 2.11          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD3  | 13       | 2.11          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD2  | 3        | 2.09          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD3  | 3        | 2.09          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD2  | 3        | 2.09          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD3  | 3        | 2.09          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD2  | 6        | 2.08          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD3  | 6        | 2.08          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD2  | 6        | 2.08          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD3  | 6        | 2.08          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD2  | 17       | 1.84          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD3  | 17       | 1.84          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD2  | 17       | 1.84          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD3  | 17       | 1.84          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD1  | 4        | 1.82          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD2  | 4        | 1.82          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD1  | 4        | 1.82          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD2  | 4        | 1.82          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD1  | 4        | 1.82          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD2  | 4        | 1.82          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD11 | 11       | 1.82          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD12 | 11       | 1.82          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD13 | 11       | 1.82          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD21 | 11       | 1.82          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD22 | 11       | 1.82          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD23 | 11       | 1.82          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 18       | 1.8           |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 18       | 1.8           |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 18       | 1.8           |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 18       | 1.8           |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 18       | 1.8           |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 18       | 1.8           |
| (1,1336) | 1:636:A:ASP:HB2 | 1:637:A:ASN:HD22 | 12       | 1.75          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 12       | 1.73          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 12       | 1.73          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 12       | 1.73          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 12       | 1.73          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 12       | 1.73          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 12       | 1.73          |
| (1,1336) | 1:636:A:ASP:HB2 | 1:637:A:ASN:HD22 | 5        | 1.73          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 4        | 1.72          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 4        | 1.72          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 4        | 1.72          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 4        | 1.72          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 4        | 1.72          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 4        | 1.72          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 11       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 11       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 11       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 11       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 11       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 11       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 13       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 13       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 13       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 13       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 13       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 13       | 1.67          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 3        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 3        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 3        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 3        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 3        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 3        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 4        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 4        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 4        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 4        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 4        | 1.66          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 4        | 1.66          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 1        | 1.65          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 1        | 1.65          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 1        | 1.65          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 1        | 1.65          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 1        | 1.65          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 1        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD11 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD12 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD13 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD21 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD22 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD23 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD11 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD12 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD13 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD21 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD22 | 5        | 1.65          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD23 | 5        | 1.65          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 5        | 1.64          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 5        | 1.64          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 5        | 1.64          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 5        | 1.64          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 5        | 1.64          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 5        | 1.64          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 7        | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 7        | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 7        | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 7        | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 7        | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 7        | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 12       | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 12       | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 12       | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 12       | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 12       | 1.59          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 12       | 1.59          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD1  | 18       | 1.58          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD2  | 18       | 1.58          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD1  | 18       | 1.58          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD2  | 18       | 1.58          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD1  | 18       | 1.58          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD2  | 18       | 1.58          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 6        | 1.58          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 6        | 1.58          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 6        | 1.58          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 6        | 1.58          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 6        | 1.58          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 6        | 1.58          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD1  | 11       | 1.57          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD2  | 11       | 1.57          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD1  | 11       | 1.57          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD2  | 11       | 1.57          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD1  | 11       | 1.57          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD2  | 11       | 1.57          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 9        | 1.53          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 9        | 1.53          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 9        | 1.53          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 9        | 1.53          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 9        | 1.53          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 9        | 1.53          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 15       | 1.52          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 15       | 1.52          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 15       | 1.52          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 15       | 1.52          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 15       | 1.52          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 15       | 1.52          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD1  | 14       | 1.52          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD2  | 14       | 1.52          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD1  | 14       | 1.52          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD2  | 14       | 1.52          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD1  | 14       | 1.52          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD2  | 14       | 1.52          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 20       | 1.51          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 20       | 1.51          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 20       | 1.51          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 20       | 1.51          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 20       | 1.51          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 20       | 1.51          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD1  | 8        | 1.5           |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD2  | 8        | 1.5           |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD1  | 8        | 1.5           |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD2  | 8        | 1.5           |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD1  | 8        | 1.5           |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD2  | 8        | 1.5           |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD11 | 13       | 1.47          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD12 | 13       | 1.47          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD13 | 13       | 1.47          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 13       | 1.47          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 13       | 1.47          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 13       | 1.47          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 16       | 1.45          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 16       | 1.45          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 16       | 1.45          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 16       | 1.45          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 16       | 1.45          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 16       | 1.45          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 12       | 1.44          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 12       | 1.44          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 12       | 1.44          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 12       | 1.44          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 12       | 1.44          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 12       | 1.44          |
| (1,994) | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 16       | 1.43          |
| (1,994) | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 16       | 1.43          |
| (1,994) | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 16       | 1.43          |
| (1,994) | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 16       | 1.43          |
| (1,994) | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 16       | 1.43          |
| (1,994) | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 16       | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 1        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 1        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 1        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 1        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 1        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 1        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 3        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 3        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 3        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 3        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 3        | 1.43          |
| (1,990) | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 3        | 1.43          |
| (1,701) | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD2  | 19       | 1.42          |
| (1,701) | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD3  | 19       | 1.42          |
| (1,701) | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD2  | 19       | 1.42          |
| (1,701) | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD3  | 19       | 1.42          |
| (1,145) | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 11       | 1.42          |
| (1,145) | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 11       | 1.42          |
| (1,145) | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 11       | 1.42          |
| (1,145) | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 11       | 1.42          |
| (1,145) | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 11       | 1.42          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 11       | 1.42          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 6        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 6        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 6        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 6        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 6        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 6        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 7        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 7        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 7        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 7        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 7        | 1.37          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 7        | 1.37          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 4        | 1.35          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 4        | 1.35          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 4        | 1.35          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 4        | 1.35          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 4        | 1.35          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 4        | 1.35          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD2  | 2        | 1.35          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD3  | 2        | 1.35          |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD2  | 2        | 1.35          |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD3  | 2        | 1.35          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 15       | 1.34          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 15       | 1.34          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 15       | 1.34          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 15       | 1.34          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 15       | 1.34          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 15       | 1.34          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 1        | 1.34          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 1        | 1.34          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 1        | 1.34          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 1        | 1.34          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 1        | 1.34          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 1        | 1.34          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 5        | 1.34          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 5        | 1.34          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 5        | 1.34          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 5        | 1.34          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 5        | 1.34          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 5        | 1.34          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD2  | 11       | 1.33          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD3  | 11       | 1.33          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD2  | 11       | 1.33          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD3  | 11       | 1.33          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 2        | 1.32          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 2        | 1.32          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 2        | 1.32          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 2        | 1.32          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 2        | 1.32          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 2        | 1.32          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD1  | 10       | 1.29          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD2  | 10       | 1.29          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD1  | 10       | 1.29          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD2  | 10       | 1.29          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD1  | 10       | 1.29          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD2  | 10       | 1.29          |
| (1,1581) | 1:656:A:ALA:HB1 | 1:659:A:ARG:HD2  | 8        | 1.25          |
| (1,1581) | 1:656:A:ALA:HB1 | 1:659:A:ARG:HD3  | 8        | 1.25          |
| (1,1581) | 1:656:A:ALA:HB2 | 1:659:A:ARG:HD2  | 8        | 1.25          |
| (1,1581) | 1:656:A:ALA:HB2 | 1:659:A:ARG:HD3  | 8        | 1.25          |
| (1,1581) | 1:656:A:ALA:HB3 | 1:659:A:ARG:HD2  | 8        | 1.25          |
| (1,1581) | 1:656:A:ALA:HB3 | 1:659:A:ARG:HD3  | 8        | 1.25          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD11 | 9        | 1.25          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD12 | 9        | 1.25          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD13 | 9        | 1.25          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD21 | 9        | 1.25          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD22 | 9        | 1.25          |
| (1,990)  | 1:590:A:SER:HB2 | 1:592:A:LEU:HD23 | 9        | 1.25          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG21 | 17       | 1.24          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG22 | 17       | 1.24          |
| (1,1514) | 1:650:A:ARG:HD2 | 1:654:A:THR:HG23 | 17       | 1.24          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG21 | 17       | 1.24          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG22 | 17       | 1.24          |
| (1,1514) | 1:650:A:ARG:HD3 | 1:654:A:THR:HG23 | 17       | 1.24          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 14       | 1.24          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 14       | 1.24          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 14       | 1.24          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 14       | 1.24          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 14       | 1.24          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 14       | 1.24          |
| (1,1581) | 1:656:A:ALA:HB1 | 1:659:A:ARG:HD2  | 17       | 1.23          |
| (1,1581) | 1:656:A:ALA:HB1 | 1:659:A:ARG:HD3  | 17       | 1.23          |
| (1,1581) | 1:656:A:ALA:HB2 | 1:659:A:ARG:HD2  | 17       | 1.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 17       | 1.23          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 17       | 1.23          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 17       | 1.23          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 5        | 1.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 5        | 1.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 5        | 1.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 5        | 1.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 5        | 1.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 5        | 1.22          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG21 | 10       | 1.21          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG22 | 10       | 1.21          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG23 | 10       | 1.21          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG21 | 10       | 1.21          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG22 | 10       | 1.21          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG23 | 10       | 1.21          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 19       | 1.21          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 19       | 1.21          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 19       | 1.21          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 19       | 1.21          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 19       | 1.21          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 19       | 1.21          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 11       | 1.21          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 11       | 1.21          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 11       | 1.21          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 11       | 1.21          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 11       | 1.21          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 11       | 1.21          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 17       | 1.18          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 17       | 1.18          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 17       | 1.18          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 17       | 1.18          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 17       | 1.18          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 17       | 1.18          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 14       | 1.16          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 14       | 1.16          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 14       | 1.16          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 14       | 1.16          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 14       | 1.16          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 14       | 1.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD11 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD12 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD13 | 6        | 1.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD21 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD22 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD23 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD11 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 6        | 1.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 6        | 1.16          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 18       | 1.15          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 18       | 1.15          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 18       | 1.15          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 18       | 1.15          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 18       | 1.15          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 18       | 1.15          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 12       | 1.15          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 12       | 1.15          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 12       | 1.15          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 12       | 1.15          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 12       | 1.15          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 12       | 1.15          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 6        | 1.14          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 6        | 1.14          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 6        | 1.14          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 6        | 1.14          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 6        | 1.14          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 6        | 1.14          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG21 | 8        | 1.14          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG22 | 8        | 1.14          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG23 | 8        | 1.14          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG21 | 8        | 1.14          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG22 | 8        | 1.14          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG23 | 8        | 1.14          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD2  | 18       | 1.14          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD3  | 18       | 1.14          |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD2  | 18       | 1.14          |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD3  | 18       | 1.14          |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD1  | 3        | 1.11          |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD2  | 3        | 1.11          |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD1  | 3        | 1.11          |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD2  | 3        | 1.11          |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD1  | 3        | 1.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,209)  | 1:542:A:MET:HE3 | 1:545:A:PHE:HD2  | 3        | 1.11          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD11 | 2        | 1.09          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD12 | 2        | 1.09          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD13 | 2        | 1.09          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD21 | 2        | 1.09          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD22 | 2        | 1.09          |
| (1,994)  | 1:590:A:SER:HB3 | 1:592:A:LEU:HD23 | 2        | 1.09          |
| (1,788)  | 1:582:A:TYR:HD1 | 1:630:A:LEU:HD11 | 16       | 1.08          |
| (1,788)  | 1:582:A:TYR:HD1 | 1:630:A:LEU:HD12 | 16       | 1.08          |
| (1,788)  | 1:582:A:TYR:HD1 | 1:630:A:LEU:HD13 | 16       | 1.08          |
| (1,788)  | 1:582:A:TYR:HD2 | 1:630:A:LEU:HD11 | 16       | 1.08          |
| (1,788)  | 1:582:A:TYR:HD2 | 1:630:A:LEU:HD12 | 16       | 1.08          |
| (1,788)  | 1:582:A:TYR:HD2 | 1:630:A:LEU:HD13 | 16       | 1.08          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD11 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD12 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD13 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD21 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD22 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD23 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD11 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD12 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD13 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD21 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD22 | 3        | 1.07          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD23 | 3        | 1.07          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD1  | 13       | 1.06          |
| (1,1484) | 1:648:A:MET:HE1 | 1:652:A:PHE:HD2  | 13       | 1.06          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD1  | 13       | 1.06          |
| (1,1484) | 1:648:A:MET:HE2 | 1:652:A:PHE:HD2  | 13       | 1.06          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD1  | 13       | 1.06          |
| (1,1484) | 1:648:A:MET:HE3 | 1:652:A:PHE:HD2  | 13       | 1.06          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD2  | 4        | 1.06          |
| (1,701)  | 1:574:A:GLU:HG2 | 1:579:A:LYS:HD3  | 4        | 1.06          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD2  | 4        | 1.06          |
| (1,701)  | 1:574:A:GLU:HG3 | 1:579:A:LYS:HD3  | 4        | 1.06          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD11 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD12 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD13 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD21 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD22 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD2 | 1:538:A:LEU:HD23 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD3 | 1:538:A:LEU:HD11 | 12       | 1.06          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 12       | 1.06          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 12       | 1.06          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 1        | 1.04          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 1        | 1.04          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 1        | 1.04          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 1        | 1.04          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 1        | 1.04          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 1        | 1.04          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 20       | 1.04          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 20       | 1.04          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 20       | 1.04          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 20       | 1.04          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 20       | 1.04          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 20       | 1.04          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 8        | 1.03          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 8        | 1.03          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 8        | 1.03          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 8        | 1.03          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 8        | 1.03          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 8        | 1.03          |
| (1,142)  | 1:538:A:LEU:HD11 | 1:586:A:HIS:H    | 12       | 1.03          |
| (1,142)  | 1:538:A:LEU:HD12 | 1:586:A:HIS:H    | 12       | 1.03          |
| (1,142)  | 1:538:A:LEU:HD13 | 1:586:A:HIS:H    | 12       | 1.03          |
| (1,142)  | 1:538:A:LEU:HD21 | 1:586:A:HIS:H    | 12       | 1.03          |
| (1,142)  | 1:538:A:LEU:HD22 | 1:586:A:HIS:H    | 12       | 1.03          |
| (1,142)  | 1:538:A:LEU:HD23 | 1:586:A:HIS:H    | 12       | 1.03          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 5        | 1.02          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 5        | 1.02          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 5        | 1.02          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 5        | 1.02          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 5        | 1.02          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 5        | 1.02          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 17       | 1.02          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 17       | 1.02          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 17       | 1.02          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 17       | 1.02          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 17       | 1.02          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 17       | 1.02          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 5        | 1.01          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 5        | 1.01          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 5        | 1.01          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 5        | 1.01          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 5        | 1.01          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 5        | 1.01          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3  | 13       | 1.0           |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3  | 13       | 1.0           |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 12       | 0.99          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 12       | 0.99          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 12       | 0.99          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 12       | 0.99          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 12       | 0.99          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 12       | 0.99          |
| (1,1476) | 1:647:A:MET:HE1  | 1:648:A:MET:HG2  | 4        | 0.99          |
| (1,1476) | 1:647:A:MET:HE1  | 1:648:A:MET:HG3  | 4        | 0.99          |
| (1,1476) | 1:647:A:MET:HE2  | 1:648:A:MET:HG2  | 4        | 0.99          |
| (1,1476) | 1:647:A:MET:HE2  | 1:648:A:MET:HG3  | 4        | 0.99          |
| (1,1476) | 1:647:A:MET:HE3  | 1:648:A:MET:HG2  | 4        | 0.99          |
| (1,1476) | 1:647:A:MET:HE3  | 1:648:A:MET:HG3  | 4        | 0.99          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 2        | 0.97          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 2        | 0.97          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 2        | 0.97          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 2        | 0.97          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 2        | 0.97          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 2        | 0.97          |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB2  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB3  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB2  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB3  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB2  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB3  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB2  | 12       | 0.97          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB3  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB2  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB3  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB2  | 12       | 0.97          |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB3  | 12       | 0.97          |
| (1,139)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HA   | 12       | 0.97          |
| (1,139)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HA   | 12       | 0.97          |
| (1,139)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HA   | 12       | 0.97          |
| (1,139)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HA   | 12       | 0.97          |
| (1,139)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HA   | 12       | 0.97          |
| (1,139)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HA   | 12       | 0.97          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 3        | 0.96          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 3        | 0.96          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 3        | 0.96          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 3        | 0.96          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 3        | 0.96          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 3        | 0.96          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD2  | 10       | 0.96          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD3  | 10       | 0.96          |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD2  | 10       | 0.96          |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD3  | 10       | 0.96          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 15       | 0.95          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 15       | 0.95          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 15       | 0.95          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 15       | 0.95          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 15       | 0.95          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 15       | 0.95          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 4        | 0.95          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 4        | 0.95          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 4        | 0.95          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 4        | 0.95          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 4        | 0.95          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 4        | 0.95          |
| (1,137)  | 1:538:A:LEU:HD11 | 1:584:A:ILE:H    | 11       | 0.94          |
| (1,137)  | 1:538:A:LEU:HD12 | 1:584:A:ILE:H    | 11       | 0.94          |
| (1,137)  | 1:538:A:LEU:HD13 | 1:584:A:ILE:H    | 11       | 0.94          |
| (1,137)  | 1:538:A:LEU:HD21 | 1:584:A:ILE:H    | 11       | 0.94          |
| (1,137)  | 1:538:A:LEU:HD22 | 1:584:A:ILE:H    | 11       | 0.94          |
| (1,137)  | 1:538:A:LEU:HD23 | 1:584:A:ILE:H    | 11       | 0.94          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 7        | 0.93          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 7        | 0.93          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 7        | 0.93          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 7        | 0.93          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 7        | 0.93          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 7        | 0.93          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 2        | 0.92          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 2        | 0.92          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 2        | 0.92          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 2        | 0.92          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 2        | 0.92          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 2        | 0.92          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 9        | 0.91          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 9        | 0.91          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 9        | 0.91          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 9        | 0.91          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 9        | 0.91          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 9        | 0.91          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 10       | 0.9           |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 10       | 0.9           |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 10       | 0.9           |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 10       | 0.9           |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 10       | 0.9           |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 10       | 0.9           |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 12       | 0.9           |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 12       | 0.9           |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 12       | 0.9           |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 12       | 0.9           |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 12       | 0.9           |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 12       | 0.9           |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 1        | 0.89          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 1        | 0.89          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 1        | 0.89          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 1        | 0.89          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 1        | 0.89          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 1        | 0.89          |
| (1,1476) | 1:647:A:MET:HE1  | 1:648:A:MET:HG2  | 12       | 0.89          |
| (1,1476) | 1:647:A:MET:HE1  | 1:648:A:MET:HG3  | 12       | 0.89          |
| (1,1476) | 1:647:A:MET:HE2  | 1:648:A:MET:HG2  | 12       | 0.89          |
| (1,1476) | 1:647:A:MET:HE2  | 1:648:A:MET:HG3  | 12       | 0.89          |
| (1,1476) | 1:647:A:MET:HE3  | 1:648:A:MET:HG2  | 12       | 0.89          |
| (1,1476) | 1:647:A:MET:HE3  | 1:648:A:MET:HG3  | 12       | 0.89          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 4        | 0.89          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 4        | 0.89          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 4        | 0.89          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 4        | 0.89          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 4        | 0.89          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 4        | 0.89          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 12       | 0.88          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 12       | 0.88          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 12       | 0.88          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 12       | 0.88          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 12       | 0.88          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 12       | 0.88          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 10       | 0.86          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 10       | 0.86          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 10       | 0.86          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 10       | 0.86          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 10       | 0.86          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 10       | 0.86          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 7        | 0.86          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 7        | 0.86          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 7        | 0.86          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 7        | 0.86          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 7        | 0.86          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 7        | 0.86          |
| (1,138)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:H    | 12       | 0.86          |
| (1,138)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:H    | 12       | 0.86          |
| (1,138)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:H    | 12       | 0.86          |
| (1,138)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:H    | 12       | 0.86          |
| (1,138)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:H    | 12       | 0.86          |
| (1,138)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:H    | 12       | 0.86          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD2  | 20       | 0.85          |
| (1,701)  | 1:574:A:GLU:HG2  | 1:579:A:LYS:HD3  | 20       | 0.85          |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD2  | 20       | 0.85          |
| (1,701)  | 1:574:A:GLU:HG3  | 1:579:A:LYS:HD3  | 20       | 0.85          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA2  | 14       | 0.84          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA3  | 14       | 0.84          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA2  | 14       | 0.84          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA3  | 14       | 0.84          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 2        | 0.83          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 2        | 0.83          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 2        | 0.83          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 2        | 0.83          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 2        | 0.83          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 2        | 0.83          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 5        | 0.82          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 5        | 0.82          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 5        | 0.82          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 5        | 0.82          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 5        | 0.82          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 5        | 0.82          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 2        | 0.82          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 2        | 0.82          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 2        | 0.82          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 2        | 0.82          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 2        | 0.82          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 2        | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 2        | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 2        | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 2        | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 2        | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 2        | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 2        | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 10       | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 10       | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 10       | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 10       | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 10       | 0.82          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 10       | 0.82          |
| (1,1043) | 1:592:A:LEU:HD11 | 1:599:A:MET:H    | 11       | 0.81          |
| (1,1043) | 1:592:A:LEU:HD12 | 1:599:A:MET:H    | 11       | 0.81          |
| (1,1043) | 1:592:A:LEU:HD13 | 1:599:A:MET:H    | 11       | 0.81          |
| (1,1043) | 1:592:A:LEU:HD21 | 1:599:A:MET:H    | 11       | 0.81          |
| (1,1043) | 1:592:A:LEU:HD22 | 1:599:A:MET:H    | 11       | 0.81          |
| (1,1043) | 1:592:A:LEU:HD23 | 1:599:A:MET:H    | 11       | 0.81          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 9        | 0.81          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 9        | 0.81          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 9        | 0.81          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 9        | 0.81          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 9        | 0.81          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 9        | 0.81          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 1        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 1        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 1        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 1        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 1        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 1        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 9        | 0.8           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 9        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 9        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 9        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 9        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 9        | 0.8           |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 13       | 0.8           |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 13       | 0.8           |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 13       | 0.8           |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 13       | 0.8           |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 13       | 0.8           |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 13       | 0.8           |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 5        | 0.79          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 5        | 0.79          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 5        | 0.79          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 5        | 0.79          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 5        | 0.79          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 5        | 0.79          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 14       | 0.79          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 14       | 0.79          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 14       | 0.79          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 14       | 0.79          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 14       | 0.79          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 14       | 0.79          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 11       | 0.78          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 11       | 0.78          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 11       | 0.78          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 11       | 0.78          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 11       | 0.78          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 11       | 0.78          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 10       | 0.78          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 10       | 0.78          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 10       | 0.78          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 10       | 0.78          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 10       | 0.78          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 10       | 0.78          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 14       | 0.78          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 14       | 0.78          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 14       | 0.78          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 14       | 0.78          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 14       | 0.78          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 14       | 0.78          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 13       | 0.77          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 13       | 0.77          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 13       | 0.77          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 13       | 0.77          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 13       | 0.77          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 13       | 0.77          |
| (1,211)  | 1:542:A:MET:HE1  | 1:606:A:TYR:HD1  | 12       | 0.77          |
| (1,211)  | 1:542:A:MET:HE1  | 1:606:A:TYR:HD2  | 12       | 0.77          |
| (1,211)  | 1:542:A:MET:HE2  | 1:606:A:TYR:HD1  | 12       | 0.77          |
| (1,211)  | 1:542:A:MET:HE2  | 1:606:A:TYR:HD2  | 12       | 0.77          |
| (1,211)  | 1:542:A:MET:HE3  | 1:606:A:TYR:HD1  | 12       | 0.77          |
| (1,211)  | 1:542:A:MET:HE3  | 1:606:A:TYR:HD2  | 12       | 0.77          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 8        | 0.76          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 8        | 0.76          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 8        | 0.76          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 8        | 0.76          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 8        | 0.76          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 8        | 0.76          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 2        | 0.76          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 2        | 0.76          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 2        | 0.76          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 2        | 0.76          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 2        | 0.76          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 2        | 0.76          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 15       | 0.75          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 15       | 0.75          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 15       | 0.75          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 15       | 0.75          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 15       | 0.75          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 15       | 0.75          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 16       | 0.75          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 16       | 0.75          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 16       | 0.75          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 16       | 0.75          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 16       | 0.75          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 16       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3  | 11       | 0.75          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3  | 11       | 0.75          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3  | 11       | 0.75          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 11       | 0.73          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 11       | 0.73          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 11       | 0.73          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 11       | 0.73          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 11       | 0.73          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 11       | 0.73          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 20       | 0.73          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 20       | 0.73          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 20       | 0.73          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 20       | 0.73          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 20       | 0.73          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 20       | 0.73          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 18       | 0.73          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 18       | 0.73          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 18       | 0.73          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 18       | 0.73          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 18       | 0.73          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 18       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 12       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 12       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 12       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 12       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 12       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 12       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 16       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 16       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 16       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 16       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 16       | 0.73          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 16       | 0.73          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 17       | 0.72          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 17       | 0.72          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 17       | 0.72          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 17       | 0.72          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 17       | 0.72          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 17       | 0.72          |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB2  | 9        | 0.72          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB3  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB2  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB3  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB2  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB3  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB2  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB3  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB2  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB3  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB2  | 9        | 0.72          |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB3  | 9        | 0.72          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 17       | 0.71          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 17       | 0.71          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 17       | 0.71          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 17       | 0.71          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 17       | 0.71          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 17       | 0.71          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 12       | 0.71          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 12       | 0.71          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 12       | 0.71          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 12       | 0.71          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 12       | 0.71          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 12       | 0.71          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 5        | 0.71          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 5        | 0.71          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 5        | 0.71          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 5        | 0.71          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 5        | 0.71          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 5        | 0.71          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 4        | 0.7           |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 4        | 0.7           |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 4        | 0.7           |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 4        | 0.7           |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 4        | 0.7           |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 4        | 0.7           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 15       | 0.7           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 15       | 0.7           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 15       | 0.7           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 15       | 0.7           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 15       | 0.7           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 15       | 0.7           |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 15       | 0.7           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 15       | 0.7           |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 15       | 0.7           |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 15       | 0.7           |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 15       | 0.7           |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 15       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD11 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD12 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD13 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD21 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD22 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD23 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD11 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 11       | 0.7           |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 11       | 0.7           |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG21 | 11       | 0.68          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG22 | 11       | 0.68          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG23 | 11       | 0.68          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG21 | 11       | 0.68          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG22 | 11       | 0.68          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG23 | 11       | 0.68          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 14       | 0.68          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 14       | 0.68          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 14       | 0.68          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 14       | 0.68          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 14       | 0.68          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 14       | 0.68          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 20       | 0.67          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 20       | 0.67          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 20       | 0.67          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 20       | 0.67          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 20       | 0.67          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 20       | 0.67          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA2  | 16       | 0.66          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA3  | 16       | 0.66          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA2  | 16       | 0.66          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA3  | 16       | 0.66          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 6        | 0.66          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 6        | 0.66          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 6        | 0.66          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 6        | 0.66          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 6        | 0.66          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 6        | 0.66          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 8        | 0.65          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 8        | 0.65          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 8        | 0.65          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 8        | 0.65          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 8        | 0.65          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 8        | 0.65          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3  | 4        | 0.64          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3  | 4        | 0.64          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 6        | 0.64          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 6        | 0.64          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 6        | 0.64          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 6        | 0.64          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 6        | 0.64          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 6        | 0.64          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1  | 16       | 0.64          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2  | 16       | 0.64          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1  | 16       | 0.64          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2  | 16       | 0.64          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1  | 16       | 0.64          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2  | 16       | 0.64          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 5        | 0.64          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 5        | 0.64          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 5        | 0.64          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 5        | 0.64          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 5        | 0.64          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 5        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD11 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD12 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD13 | 1        | 0.64          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD21 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD22 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD23 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD11 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 1        | 0.64          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 1        | 0.64          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD11 | 17       | 0.63          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD12 | 17       | 0.63          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD13 | 17       | 0.63          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD21 | 17       | 0.63          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD22 | 17       | 0.63          |
| (1,990)  | 1:590:A:SER:HB2  | 1:592:A:LEU:HD23 | 17       | 0.63          |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG2  | 15       | 0.63          |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG3  | 15       | 0.63          |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG2  | 15       | 0.63          |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG3  | 15       | 0.63          |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG2  | 15       | 0.63          |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG3  | 15       | 0.63          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 13       | 0.62          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 13       | 0.62          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 13       | 0.62          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 13       | 0.62          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 13       | 0.62          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 13       | 0.62          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG21 | 13       | 0.62          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG22 | 13       | 0.62          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG23 | 13       | 0.62          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG21 | 13       | 0.62          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG22 | 13       | 0.62          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG23 | 13       | 0.62          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1  | 18       | 0.62          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2  | 18       | 0.62          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3  | 18       | 0.62          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1  | 18       | 0.62          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2  | 18       | 0.62          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3  | 18       | 0.62          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2  | 9        | 0.61          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3  | 9        | 0.61          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3  | 9        | 0.61          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA2  | 1        | 0.61          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA3  | 1        | 0.61          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA2  | 1        | 0.61          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA3  | 1        | 0.61          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA2  | 15       | 0.61          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA3  | 15       | 0.61          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA2  | 15       | 0.61          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA3  | 15       | 0.61          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 4        | 0.61          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 4        | 0.61          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 4        | 0.61          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 4        | 0.61          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 4        | 0.61          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 4        | 0.61          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 6        | 0.61          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 6        | 0.61          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 6        | 0.61          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 6        | 0.61          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 6        | 0.61          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 6        | 0.61          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 3        | 0.6           |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 3        | 0.6           |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 3        | 0.6           |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 3        | 0.6           |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 3        | 0.6           |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 3        | 0.6           |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD1  | 7        | 0.6           |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD2  | 7        | 0.6           |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD1  | 7        | 0.6           |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD2  | 7        | 0.6           |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD1  | 7        | 0.6           |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD2  | 7        | 0.6           |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 2        | 0.59          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3 | 2        | 0.59          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2 | 2        | 0.59          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3 | 2        | 0.59          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2 | 2        | 0.59          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3 | 2        | 0.59          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1 | 9        | 0.59          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2 | 9        | 0.59          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1 | 9        | 0.59          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2 | 9        | 0.59          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1 | 9        | 0.59          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2 | 9        | 0.59          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H   | 16       | 0.59          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H   | 16       | 0.59          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H   | 16       | 0.59          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H   | 16       | 0.59          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H   | 16       | 0.59          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H   | 16       | 0.59          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1 | 11       | 0.59          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2 | 11       | 0.59          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1 | 11       | 0.59          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2 | 11       | 0.59          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1 | 11       | 0.59          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2 | 11       | 0.59          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB1 | 4        | 0.58          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB2 | 4        | 0.58          |
| (1,1513) | 1:650:A:ARG:HD2  | 1:651:A:ALA:HB3 | 4        | 0.58          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB1 | 4        | 0.58          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB2 | 4        | 0.58          |
| (1,1513) | 1:650:A:ARG:HD3  | 1:651:A:ALA:HB3 | 4        | 0.58          |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2 | 10       | 0.58          |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2 | 10       | 0.58          |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2 | 10       | 0.58          |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2 | 10       | 0.58          |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2 | 10       | 0.58          |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2 | 10       | 0.58          |
| (1,136)  | 1:538:A:LEU:HD11 | 1:541:A:SER:H   | 12       | 0.58          |
| (1,136)  | 1:538:A:LEU:HD12 | 1:541:A:SER:H   | 12       | 0.58          |
| (1,136)  | 1:538:A:LEU:HD13 | 1:541:A:SER:H   | 12       | 0.58          |
| (1,136)  | 1:538:A:LEU:HD21 | 1:541:A:SER:H   | 12       | 0.58          |
| (1,136)  | 1:538:A:LEU:HD22 | 1:541:A:SER:H   | 12       | 0.58          |
| (1,136)  | 1:538:A:LEU:HD23 | 1:541:A:SER:H   | 12       | 0.58          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2 | 14       | 0.57          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 14       | 0.57          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 14       | 0.57          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 14       | 0.57          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 14       | 0.57          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 14       | 0.57          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 12       | 0.57          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 12       | 0.57          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 12       | 0.57          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 12       | 0.57          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 12       | 0.57          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 12       | 0.57          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 3        | 0.56          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 3        | 0.56          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 3        | 0.56          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 3        | 0.56          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 3        | 0.56          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 3        | 0.56          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 12       | 0.56          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 12       | 0.56          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 12       | 0.56          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 12       | 0.56          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 12       | 0.56          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 12       | 0.56          |
| (1,139)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HA   | 9        | 0.56          |
| (1,139)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HA   | 9        | 0.56          |
| (1,139)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HA   | 9        | 0.56          |
| (1,139)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HA   | 9        | 0.56          |
| (1,139)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HA   | 9        | 0.56          |
| (1,139)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HA   | 9        | 0.56          |
| (1,137)  | 1:538:A:LEU:HD11 | 1:584:A:ILE:H    | 12       | 0.56          |
| (1,137)  | 1:538:A:LEU:HD12 | 1:584:A:ILE:H    | 12       | 0.56          |
| (1,137)  | 1:538:A:LEU:HD13 | 1:584:A:ILE:H    | 12       | 0.56          |
| (1,137)  | 1:538:A:LEU:HD21 | 1:584:A:ILE:H    | 12       | 0.56          |
| (1,137)  | 1:538:A:LEU:HD22 | 1:584:A:ILE:H    | 12       | 0.56          |
| (1,137)  | 1:538:A:LEU:HD23 | 1:584:A:ILE:H    | 12       | 0.56          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD11 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD12 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD13 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD21 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD22 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD23 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD11 | 7        | 0.56          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 7        | 0.56          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 7        | 0.56          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 7        | 0.55          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 7        | 0.55          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 7        | 0.55          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 7        | 0.55          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 7        | 0.55          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 7        | 0.55          |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 8        | 0.55          |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 8        | 0.55          |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 8        | 0.55          |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 8        | 0.55          |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 8        | 0.55          |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 8        | 0.55          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 10       | 0.55          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 10       | 0.55          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 10       | 0.55          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 10       | 0.55          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 10       | 0.55          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 10       | 0.55          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 18       | 0.55          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 18       | 0.55          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 18       | 0.55          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 18       | 0.55          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 18       | 0.55          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 18       | 0.55          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 4        | 0.55          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 4        | 0.55          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 4        | 0.55          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 4        | 0.55          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 4        | 0.55          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 4        | 0.55          |
| (1,142)  | 1:538:A:LEU:HD11 | 1:586:A:HIS:H    | 9        | 0.55          |
| (1,142)  | 1:538:A:LEU:HD12 | 1:586:A:HIS:H    | 9        | 0.55          |
| (1,142)  | 1:538:A:LEU:HD13 | 1:586:A:HIS:H    | 9        | 0.55          |
| (1,142)  | 1:538:A:LEU:HD21 | 1:586:A:HIS:H    | 9        | 0.55          |
| (1,142)  | 1:538:A:LEU:HD22 | 1:586:A:HIS:H    | 9        | 0.55          |
| (1,142)  | 1:538:A:LEU:HD23 | 1:586:A:HIS:H    | 9        | 0.55          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 15       | 0.54          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 15       | 0.54          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 15       | 0.54          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 15       | 0.54          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 15       | 0.54          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 15       | 0.54          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 6        | 0.54          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 6        | 0.54          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 6        | 0.54          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 6        | 0.54          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 6        | 0.54          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 6        | 0.54          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA2  | 4        | 0.54          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA3  | 4        | 0.54          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA2  | 4        | 0.54          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA3  | 4        | 0.54          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 13       | 0.54          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 13       | 0.54          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 13       | 0.54          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 13       | 0.54          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 13       | 0.54          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 13       | 0.54          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 8        | 0.54          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 8        | 0.54          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 8        | 0.54          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 8        | 0.54          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 8        | 0.54          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 8        | 0.54          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD1  | 5        | 0.54          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD2  | 5        | 0.54          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD1  | 5        | 0.54          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD2  | 5        | 0.54          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 2        | 0.53          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 2        | 0.53          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 2        | 0.53          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 2        | 0.53          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 9        | 0.53          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 9        | 0.53          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 9        | 0.53          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 9        | 0.53          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 9        | 0.53          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 9        | 0.53          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD11 | 19       | 0.53          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD12 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD13 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD21 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD22 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD23 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD11 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 19       | 0.53          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 19       | 0.53          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 8        | 0.52          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 8        | 0.52          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 8        | 0.52          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 8        | 0.52          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 8        | 0.52          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 8        | 0.52          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 12       | 0.51          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 12       | 0.51          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 12       | 0.51          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 12       | 0.51          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 3        | 0.51          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 3        | 0.51          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 3        | 0.51          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 3        | 0.51          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 3        | 0.51          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 3        | 0.51          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 6        | 0.5           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 6        | 0.5           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 6        | 0.5           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 6        | 0.5           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 6        | 0.5           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 6        | 0.5           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 7        | 0.5           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 7        | 0.5           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 7        | 0.5           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 7        | 0.5           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 7        | 0.5           |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 7        | 0.5           |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1  | 9        | 0.49          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2  | 9        | 0.49          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1  | 9        | 0.49          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2  | 9        | 0.49          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1  | 9        | 0.49          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2  | 9        | 0.49          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA2  | 7        | 0.49          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA3  | 7        | 0.49          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA2  | 7        | 0.49          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA3  | 7        | 0.49          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA2  | 8        | 0.49          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA3  | 8        | 0.49          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA2  | 8        | 0.49          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA3  | 8        | 0.49          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 8        | 0.49          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 8        | 0.49          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 8        | 0.49          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 8        | 0.49          |
| (1,138)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:H    | 9        | 0.49          |
| (1,138)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:H    | 9        | 0.49          |
| (1,138)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:H    | 9        | 0.49          |
| (1,138)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:H    | 9        | 0.49          |
| (1,138)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:H    | 9        | 0.49          |
| (1,138)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:H    | 9        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD11 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD12 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD13 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD21 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD22 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD23 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD11 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 8        | 0.49          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 8        | 0.49          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 1        | 0.48          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 1        | 0.48          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 1        | 0.48          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 1        | 0.48          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 4        | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 4        | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 4        | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 4        | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 4        | 0.47          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 4        | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 17       | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 17       | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 17       | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 17       | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 17       | 0.47          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 17       | 0.47          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 4        | 0.47          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 4        | 0.47          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 4        | 0.47          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 4        | 0.47          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 18       | 0.47          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 18       | 0.47          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 18       | 0.47          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 18       | 0.47          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA2  | 13       | 0.47          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA3  | 13       | 0.47          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA2  | 13       | 0.47          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA3  | 13       | 0.47          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 1        | 0.46          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 1        | 0.46          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 1        | 0.46          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 1        | 0.46          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 1        | 0.46          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 1        | 0.46          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 3        | 0.46          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 3        | 0.46          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 3        | 0.46          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 3        | 0.46          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 20       | 0.46          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 20       | 0.46          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 20       | 0.46          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 20       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HB2  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HB3  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HB2  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HB3  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HB2  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HB3  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HB2  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HB3  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HB2  | 11       | 0.46          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1042) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HB3  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HB2  | 11       | 0.46          |
| (1,1042) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HB3  | 11       | 0.46          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 18       | 0.46          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 18       | 0.46          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 18       | 0.46          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 18       | 0.46          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 18       | 0.46          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 18       | 0.46          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 6        | 0.46          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 6        | 0.46          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 6        | 0.46          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 6        | 0.46          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 6        | 0.46          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 6        | 0.46          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 11       | 0.45          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 11       | 0.45          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 11       | 0.45          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 11       | 0.45          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 11       | 0.45          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 11       | 0.45          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 19       | 0.45          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 19       | 0.45          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 19       | 0.45          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 19       | 0.45          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 19       | 0.45          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 19       | 0.45          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA2  | 10       | 0.45          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA3  | 10       | 0.45          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA2  | 10       | 0.45          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA3  | 10       | 0.45          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 18       | 0.45          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 18       | 0.45          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 18       | 0.45          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 18       | 0.45          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 2        | 0.45          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 2        | 0.45          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 2        | 0.45          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 2        | 0.45          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 2        | 0.45          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 2        | 0.45          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 5        | 0.45          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 5        | 0.45          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 5        | 0.45          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 5        | 0.45          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 5        | 0.45          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 5        | 0.45          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 15       | 0.45          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 15       | 0.45          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 15       | 0.45          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 15       | 0.45          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 15       | 0.45          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 15       | 0.45          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 17       | 0.44          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 17       | 0.44          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 17       | 0.44          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 17       | 0.44          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 17       | 0.44          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 17       | 0.44          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1  | 15       | 0.44          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2  | 15       | 0.44          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1  | 15       | 0.44          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2  | 15       | 0.44          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1  | 15       | 0.44          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2  | 15       | 0.44          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 6        | 0.44          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 6        | 0.44          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 6        | 0.44          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 6        | 0.44          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 6        | 0.44          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 6        | 0.44          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 19       | 0.43          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 19       | 0.43          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 19       | 0.43          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 19       | 0.43          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 19       | 0.43          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 19       | 0.43          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 6        | 0.43          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 6        | 0.43          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 6        | 0.43          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 6        | 0.43          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 6        | 0.43          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 6        | 0.43          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 5        | 0.43          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 5        | 0.43          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 5        | 0.43          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 5        | 0.43          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 5        | 0.43          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 5        | 0.43          |
| (1,1608) | 1:662:A:ARG:HB2  | 1:662:A:ARG:HD2  | 7        | 0.42          |
| (1,1608) | 1:662:A:ARG:HB2  | 1:662:A:ARG:HD3  | 7        | 0.42          |
| (1,1608) | 1:662:A:ARG:HB3  | 1:662:A:ARG:HD2  | 7        | 0.42          |
| (1,1608) | 1:662:A:ARG:HB3  | 1:662:A:ARG:HD3  | 7        | 0.42          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 5        | 0.42          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 5        | 0.42          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 5        | 0.42          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 5        | 0.42          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 16       | 0.42          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 16       | 0.42          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 16       | 0.42          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 16       | 0.42          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 16       | 0.42          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 16       | 0.42          |
| (1,455)  | 1:560:A:LEU:HD11 | 1:631:A:TYR:HD1  | 5        | 0.42          |
| (1,455)  | 1:560:A:LEU:HD11 | 1:631:A:TYR:HD2  | 5        | 0.42          |
| (1,455)  | 1:560:A:LEU:HD12 | 1:631:A:TYR:HD1  | 5        | 0.42          |
| (1,455)  | 1:560:A:LEU:HD12 | 1:631:A:TYR:HD2  | 5        | 0.42          |
| (1,455)  | 1:560:A:LEU:HD13 | 1:631:A:TYR:HD1  | 5        | 0.42          |
| (1,455)  | 1:560:A:LEU:HD13 | 1:631:A:TYR:HD2  | 5        | 0.42          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 16       | 0.42          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 16       | 0.42          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 16       | 0.42          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 16       | 0.42          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 16       | 0.42          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 16       | 0.42          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG21 | 6        | 0.41          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG22 | 6        | 0.41          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG23 | 6        | 0.41          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG21 | 6        | 0.41          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG22 | 6        | 0.41          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG23 | 6        | 0.41          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1  | 14       | 0.41          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2  | 14       | 0.41          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1  | 14       | 0.41          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2  | 14       | 0.41          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1  | 14       | 0.41          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2  | 14       | 0.41          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA2  | 5        | 0.41          |
| (1,699)  | 1:574:A:GLU:HG2  | 1:575:A:GLY:HA3  | 5        | 0.41          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA2  | 5        | 0.41          |
| (1,699)  | 1:574:A:GLU:HG3  | 1:575:A:GLY:HA3  | 5        | 0.41          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 17       | 0.41          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 17       | 0.41          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 17       | 0.41          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 17       | 0.41          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 17       | 0.41          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 17       | 0.41          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 3        | 0.4           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 3        | 0.4           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 3        | 0.4           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 3        | 0.4           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 3        | 0.4           |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 3        | 0.4           |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 7        | 0.4           |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 7        | 0.4           |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 7        | 0.4           |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 7        | 0.4           |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 7        | 0.4           |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 7        | 0.4           |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1  | 8        | 0.4           |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2  | 8        | 0.4           |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1  | 8        | 0.4           |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2  | 8        | 0.4           |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1  | 8        | 0.4           |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2  | 8        | 0.4           |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1  | 19       | 0.4           |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2  | 19       | 0.4           |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1  | 19       | 0.4           |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2  | 19       | 0.4           |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1  | 19       | 0.4           |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2  | 19       | 0.4           |
| (1,137)  | 1:538:A:LEU:HD11 | 1:584:A:ILE:H    | 18       | 0.4           |
| (1,137)  | 1:538:A:LEU:HD12 | 1:584:A:ILE:H    | 18       | 0.4           |
| (1,137)  | 1:538:A:LEU:HD13 | 1:584:A:ILE:H    | 18       | 0.4           |
| (1,137)  | 1:538:A:LEU:HD21 | 1:584:A:ILE:H    | 18       | 0.4           |
| (1,137)  | 1:538:A:LEU:HD22 | 1:584:A:ILE:H    | 18       | 0.4           |
| (1,137)  | 1:538:A:LEU:HD23 | 1:584:A:ILE:H    | 18       | 0.4           |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2  | 12       | 0.39          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3 | 12       | 0.39          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3 | 12       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB2 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB3 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB2 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB3 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB2 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB3 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB2 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB3 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB2 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB3 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB2 | 11       | 0.39          |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB3 | 11       | 0.39          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2 | 5        | 0.38          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3 | 5        | 0.38          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2 | 5        | 0.38          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3 | 5        | 0.38          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2 | 5        | 0.38          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3 | 5        | 0.38          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3 | 16       | 0.38          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3 | 16       | 0.38          |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2 | 2        | 0.38          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 2        | 0.38          |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 2        | 0.38          |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 2        | 0.38          |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 2        | 0.38          |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 2        | 0.38          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H    | 7        | 0.38          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H    | 7        | 0.38          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H    | 7        | 0.38          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H    | 7        | 0.38          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H    | 7        | 0.38          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H    | 7        | 0.38          |
| (1,932)  | 1:588:A:VAL:HG11 | 1:602:A:SER:HB3  | 18       | 0.38          |
| (1,932)  | 1:588:A:VAL:HG12 | 1:602:A:SER:HB3  | 18       | 0.38          |
| (1,932)  | 1:588:A:VAL:HG13 | 1:602:A:SER:HB3  | 18       | 0.38          |
| (1,932)  | 1:588:A:VAL:HG21 | 1:602:A:SER:HB3  | 18       | 0.38          |
| (1,932)  | 1:588:A:VAL:HG22 | 1:602:A:SER:HB3  | 18       | 0.38          |
| (1,932)  | 1:588:A:VAL:HG23 | 1:602:A:SER:HB3  | 18       | 0.38          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 17       | 0.38          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 17       | 0.38          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 17       | 0.38          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 17       | 0.38          |
| (1,138)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:H    | 11       | 0.38          |
| (1,138)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:H    | 11       | 0.38          |
| (1,138)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:H    | 11       | 0.38          |
| (1,138)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:H    | 11       | 0.38          |
| (1,138)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:H    | 11       | 0.38          |
| (1,138)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:H    | 11       | 0.38          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 7        | 0.37          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 7        | 0.37          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 7        | 0.37          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 7        | 0.37          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 7        | 0.37          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 7        | 0.37          |
| (1,1031) | 1:592:A:LEU:HA   | 1:592:A:LEU:HD11 | 11       | 0.37          |
| (1,1031) | 1:592:A:LEU:HA   | 1:592:A:LEU:HD12 | 11       | 0.37          |
| (1,1031) | 1:592:A:LEU:HA   | 1:592:A:LEU:HD13 | 11       | 0.37          |
| (1,1031) | 1:592:A:LEU:HA   | 1:592:A:LEU:HD21 | 11       | 0.37          |
| (1,1031) | 1:592:A:LEU:HA   | 1:592:A:LEU:HD22 | 11       | 0.37          |
| (1,1031) | 1:592:A:LEU:HA   | 1:592:A:LEU:HD23 | 11       | 0.37          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 13       | 0.37          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 13       | 0.37          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 13       | 0.37          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 13       | 0.37          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 13       | 0.37          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 13       | 0.37          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 17       | 0.37          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 17       | 0.37          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 17       | 0.37          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 17       | 0.37          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 17       | 0.37          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 17       | 0.37          |
| (1,137)  | 1:538:A:LEU:HD11 | 1:584:A:ILE:H    | 17       | 0.37          |
| (1,137)  | 1:538:A:LEU:HD12 | 1:584:A:ILE:H    | 17       | 0.37          |
| (1,137)  | 1:538:A:LEU:HD13 | 1:584:A:ILE:H    | 17       | 0.37          |
| (1,137)  | 1:538:A:LEU:HD21 | 1:584:A:ILE:H    | 17       | 0.37          |
| (1,137)  | 1:538:A:LEU:HD22 | 1:584:A:ILE:H    | 17       | 0.37          |
| (1,137)  | 1:538:A:LEU:HD23 | 1:584:A:ILE:H    | 17       | 0.37          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 8        | 0.36          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 8        | 0.36          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 8        | 0.36          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 8        | 0.36          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 14       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 14       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 14       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 14       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 16       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 16       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 16       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 16       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 19       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 19       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 19       | 0.36          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 19       | 0.36          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD1  | 15       | 0.36          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD2  | 15       | 0.36          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD1  | 15       | 0.36          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD2  | 15       | 0.36          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 15       | 0.36          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 15       | 0.36          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 15       | 0.36          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 15       | 0.36          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 15       | 0.36          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 15       | 0.36          |
| (1,211)  | 1:542:A:MET:HE1  | 1:606:A:TYR:HD1  | 9        | 0.36          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,211)  | 1:542:A:MET:HE1  | 1:606:A:TYR:HD2  | 9        | 0.36          |
| (1,211)  | 1:542:A:MET:HE2  | 1:606:A:TYR:HD1  | 9        | 0.36          |
| (1,211)  | 1:542:A:MET:HE2  | 1:606:A:TYR:HD2  | 9        | 0.36          |
| (1,211)  | 1:542:A:MET:HE3  | 1:606:A:TYR:HD1  | 9        | 0.36          |
| (1,211)  | 1:542:A:MET:HE3  | 1:606:A:TYR:HD2  | 9        | 0.36          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG21 | 9        | 0.35          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG22 | 9        | 0.35          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG23 | 9        | 0.35          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG21 | 9        | 0.35          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG22 | 9        | 0.35          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG23 | 9        | 0.35          |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 14       | 0.34          |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 14       | 0.34          |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 14       | 0.34          |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 14       | 0.34          |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 14       | 0.34          |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 14       | 0.34          |
| (1,968)  | 1:589:A:VAL:HG21 | 1:607:A:PHE:HD1  | 12       | 0.34          |
| (1,968)  | 1:589:A:VAL:HG21 | 1:607:A:PHE:HD2  | 12       | 0.34          |
| (1,968)  | 1:589:A:VAL:HG22 | 1:607:A:PHE:HD1  | 12       | 0.34          |
| (1,968)  | 1:589:A:VAL:HG22 | 1:607:A:PHE:HD2  | 12       | 0.34          |
| (1,968)  | 1:589:A:VAL:HG23 | 1:607:A:PHE:HD1  | 12       | 0.34          |
| (1,968)  | 1:589:A:VAL:HG23 | 1:607:A:PHE:HD2  | 12       | 0.34          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 1        | 0.34          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 1        | 0.34          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 1        | 0.34          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 1        | 0.34          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 1        | 0.34          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 1        | 0.34          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 10       | 0.34          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 10       | 0.34          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 10       | 0.34          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 10       | 0.34          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 10       | 0.34          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 10       | 0.34          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 1        | 0.34          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 1        | 0.34          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 1        | 0.34          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 1        | 0.34          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 1        | 0.34          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 1        | 0.34          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 18       | 0.33          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 18       | 0.33          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 18       | 0.33          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 18       | 0.33          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 18       | 0.33          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 18       | 0.33          |
| (1,932)  | 1:588:A:VAL:HG11 | 1:602:A:SER:HB3  | 6        | 0.33          |
| (1,932)  | 1:588:A:VAL:HG12 | 1:602:A:SER:HB3  | 6        | 0.33          |
| (1,932)  | 1:588:A:VAL:HG13 | 1:602:A:SER:HB3  | 6        | 0.33          |
| (1,932)  | 1:588:A:VAL:HG21 | 1:602:A:SER:HB3  | 6        | 0.33          |
| (1,932)  | 1:588:A:VAL:HG22 | 1:602:A:SER:HB3  | 6        | 0.33          |
| (1,932)  | 1:588:A:VAL:HG23 | 1:602:A:SER:HB3  | 6        | 0.33          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 19       | 0.33          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 19       | 0.33          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 19       | 0.33          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 19       | 0.33          |
| (1,137)  | 1:538:A:LEU:HD11 | 1:584:A:ILE:H    | 4        | 0.33          |
| (1,137)  | 1:538:A:LEU:HD12 | 1:584:A:ILE:H    | 4        | 0.33          |
| (1,137)  | 1:538:A:LEU:HD13 | 1:584:A:ILE:H    | 4        | 0.33          |
| (1,137)  | 1:538:A:LEU:HD21 | 1:584:A:ILE:H    | 4        | 0.33          |
| (1,137)  | 1:538:A:LEU:HD22 | 1:584:A:ILE:H    | 4        | 0.33          |
| (1,137)  | 1:538:A:LEU:HD23 | 1:584:A:ILE:H    | 4        | 0.33          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD1  | 12       | 0.32          |
| (1,1484) | 1:648:A:MET:HE1  | 1:652:A:PHE:HD2  | 12       | 0.32          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD1  | 12       | 0.32          |
| (1,1484) | 1:648:A:MET:HE2  | 1:652:A:PHE:HD2  | 12       | 0.32          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD1  | 12       | 0.32          |
| (1,1484) | 1:648:A:MET:HE3  | 1:652:A:PHE:HD2  | 12       | 0.32          |
| (1,968)  | 1:589:A:VAL:HG21 | 1:607:A:PHE:HD1  | 14       | 0.32          |
| (1,968)  | 1:589:A:VAL:HG21 | 1:607:A:PHE:HD2  | 14       | 0.32          |
| (1,968)  | 1:589:A:VAL:HG22 | 1:607:A:PHE:HD1  | 14       | 0.32          |
| (1,968)  | 1:589:A:VAL:HG22 | 1:607:A:PHE:HD2  | 14       | 0.32          |
| (1,968)  | 1:589:A:VAL:HG23 | 1:607:A:PHE:HD1  | 14       | 0.32          |
| (1,968)  | 1:589:A:VAL:HG23 | 1:607:A:PHE:HD2  | 14       | 0.32          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 4        | 0.32          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 4        | 0.32          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 4        | 0.32          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 4        | 0.32          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 4        | 0.32          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 4        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 3        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 3        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 3        | 0.32          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 3        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 3        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 3        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 8        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 8        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 8        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 8        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 8        | 0.32          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 8        | 0.32          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 7        | 0.31          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 7        | 0.31          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 7        | 0.31          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 7        | 0.31          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 7        | 0.31          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 7        | 0.31          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 9        | 0.31          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 9        | 0.31          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 9        | 0.31          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 9        | 0.31          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 9        | 0.31          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 9        | 0.31          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 7        | 0.31          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 7        | 0.31          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 7        | 0.31          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 7        | 0.31          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 7        | 0.31          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 7        | 0.31          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA2  | 17       | 0.3           |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA3  | 17       | 0.3           |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA2  | 17       | 0.3           |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA3  | 17       | 0.3           |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 17       | 0.3           |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 17       | 0.3           |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 17       | 0.3           |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 17       | 0.3           |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 17       | 0.3           |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 17       | 0.3           |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 9        | 0.3           |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 9        | 0.3           |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 9        | 0.3           |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 9        | 0.3           |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 9        | 0.3           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 9        | 0.3           |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD1  | 2        | 0.3           |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD2  | 2        | 0.3           |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD1  | 2        | 0.3           |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD2  | 2        | 0.3           |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 15       | 0.3           |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 15       | 0.3           |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 15       | 0.3           |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 15       | 0.3           |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 14       | 0.29          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 14       | 0.29          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 14       | 0.29          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 14       | 0.29          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 14       | 0.29          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 14       | 0.29          |
| (1,932)  | 1:588:A:VAL:HG11 | 1:602:A:SER:HB3  | 7        | 0.29          |
| (1,932)  | 1:588:A:VAL:HG12 | 1:602:A:SER:HB3  | 7        | 0.29          |
| (1,932)  | 1:588:A:VAL:HG13 | 1:602:A:SER:HB3  | 7        | 0.29          |
| (1,932)  | 1:588:A:VAL:HG21 | 1:602:A:SER:HB3  | 7        | 0.29          |
| (1,932)  | 1:588:A:VAL:HG22 | 1:602:A:SER:HB3  | 7        | 0.29          |
| (1,932)  | 1:588:A:VAL:HG23 | 1:602:A:SER:HB3  | 7        | 0.29          |
| (1,932)  | 1:588:A:VAL:HG11 | 1:602:A:SER:HB3  | 13       | 0.29          |
| (1,932)  | 1:588:A:VAL:HG12 | 1:602:A:SER:HB3  | 13       | 0.29          |
| (1,932)  | 1:588:A:VAL:HG13 | 1:602:A:SER:HB3  | 13       | 0.29          |
| (1,932)  | 1:588:A:VAL:HG21 | 1:602:A:SER:HB3  | 13       | 0.29          |
| (1,932)  | 1:588:A:VAL:HG22 | 1:602:A:SER:HB3  | 13       | 0.29          |
| (1,932)  | 1:588:A:VAL:HG23 | 1:602:A:SER:HB3  | 13       | 0.29          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD11 | 13       | 0.29          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD12 | 13       | 0.29          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD13 | 13       | 0.29          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD21 | 13       | 0.29          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD22 | 13       | 0.29          |
| (1,449)  | 1:560:A:LEU:HA   | 1:633:A:LEU:HD23 | 13       | 0.29          |
| (1,142)  | 1:538:A:LEU:HD11 | 1:586:A:HIS:H    | 11       | 0.29          |
| (1,142)  | 1:538:A:LEU:HD12 | 1:586:A:HIS:H    | 11       | 0.29          |
| (1,142)  | 1:538:A:LEU:HD13 | 1:586:A:HIS:H    | 11       | 0.29          |
| (1,142)  | 1:538:A:LEU:HD21 | 1:586:A:HIS:H    | 11       | 0.29          |
| (1,142)  | 1:538:A:LEU:HD22 | 1:586:A:HIS:H    | 11       | 0.29          |
| (1,142)  | 1:538:A:LEU:HD23 | 1:586:A:HIS:H    | 11       | 0.29          |
| (1,1612) | 1:663:A:ILE:HA   | 1:663:A:ILE:HG12 | 8        | 0.27          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD2  | 12       | 0.27          |
| (1,1581) | 1:656:A:ALA:HB1  | 1:659:A:ARG:HD3  | 12       | 0.27          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD2  | 12       | 0.27          |
| (1,1581) | 1:656:A:ALA:HB2  | 1:659:A:ARG:HD3  | 12       | 0.27          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD2  | 12       | 0.27          |
| (1,1581) | 1:656:A:ALA:HB3  | 1:659:A:ARG:HD3  | 12       | 0.27          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1  | 13       | 0.27          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2  | 13       | 0.27          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1  | 13       | 0.27          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2  | 13       | 0.27          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1  | 13       | 0.27          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2  | 13       | 0.27          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 16       | 0.27          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 16       | 0.27          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 16       | 0.27          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 16       | 0.27          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 16       | 0.27          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 16       | 0.27          |
| (1,1612) | 1:663:A:ILE:HA   | 1:663:A:ILE:HG12 | 20       | 0.26          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 19       | 0.26          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 19       | 0.26          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 19       | 0.26          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 19       | 0.26          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 19       | 0.26          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 19       | 0.26          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 8        | 0.26          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 8        | 0.26          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 8        | 0.26          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 8        | 0.26          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 8        | 0.26          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 8        | 0.26          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 8        | 0.26          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 8        | 0.26          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 8        | 0.26          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 8        | 0.26          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 8        | 0.26          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 8        | 0.26          |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD1  | 16       | 0.26          |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD2  | 16       | 0.26          |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD1  | 16       | 0.26          |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD2  | 16       | 0.26          |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD1  | 16       | 0.26          |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD2  | 16       | 0.26          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 13       | 0.26          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 13       | 0.26          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 13       | 0.26          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 13       | 0.26          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 13       | 0.26          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 13       | 0.26          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG21 | 14       | 0.25          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG22 | 14       | 0.25          |
| (1,1514) | 1:650:A:ARG:HD2  | 1:654:A:THR:HG23 | 14       | 0.25          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG21 | 14       | 0.25          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG22 | 14       | 0.25          |
| (1,1514) | 1:650:A:ARG:HD3  | 1:654:A:THR:HG23 | 14       | 0.25          |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD2  | 6        | 0.25          |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD3  | 6        | 0.25          |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD2  | 6        | 0.25          |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD3  | 6        | 0.25          |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD2  | 13       | 0.25          |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD3  | 13       | 0.25          |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD2  | 13       | 0.25          |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD3  | 13       | 0.25          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA2  | 9        | 0.25          |
| (1,1072) | 1:594:A:LYS:HD2  | 1:595:A:GLY:HA3  | 9        | 0.25          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA2  | 9        | 0.25          |
| (1,1072) | 1:594:A:LYS:HD3  | 1:595:A:GLY:HA3  | 9        | 0.25          |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 9        | 0.25          |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 9        | 0.25          |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 9        | 0.25          |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 9        | 0.25          |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 9        | 0.25          |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 9        | 0.25          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 6        | 0.25          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 6        | 0.25          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 6        | 0.25          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 6        | 0.25          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 6        | 0.25          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 6        | 0.25          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 17       | 0.25          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 17       | 0.25          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 17       | 0.25          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 17       | 0.25          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 17       | 0.25          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 17       | 0.25          |
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD1  | 10       | 0.25          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,209)  | 1:542:A:MET:HE1  | 1:545:A:PHE:HD2 | 10       | 0.25          |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD1 | 10       | 0.25          |
| (1,209)  | 1:542:A:MET:HE2  | 1:545:A:PHE:HD2 | 10       | 0.25          |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD1 | 10       | 0.25          |
| (1,209)  | 1:542:A:MET:HE3  | 1:545:A:PHE:HD2 | 10       | 0.25          |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG2 | 3        | 0.25          |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG3 | 3        | 0.25          |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG2 | 3        | 0.25          |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG3 | 3        | 0.25          |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG2 | 3        | 0.25          |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG3 | 3        | 0.25          |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB2 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HB3 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB2 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HB3 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB2 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HB3 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB2 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HB3 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB2 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HB3 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB2 | 16       | 0.25          |
| (1,141)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HB3 | 16       | 0.25          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3 | 6        | 0.24          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3 | 14       | 0.24          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3 | 14       | 0.24          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3 | 14       | 0.24          |
| (1,1043) | 1:592:A:LEU:HD11 | 1:599:A:MET:H   | 10       | 0.24          |
| (1,1043) | 1:592:A:LEU:HD12 | 1:599:A:MET:H   | 10       | 0.24          |
| (1,1043) | 1:592:A:LEU:HD13 | 1:599:A:MET:H   | 10       | 0.24          |
| (1,1043) | 1:592:A:LEU:HD21 | 1:599:A:MET:H   | 10       | 0.24          |
| (1,1043) | 1:592:A:LEU:HD22 | 1:599:A:MET:H   | 10       | 0.24          |
| (1,1043) | 1:592:A:LEU:HD23 | 1:599:A:MET:H   | 10       | 0.24          |
| (1,1039) | 1:592:A:LEU:HD11 | 1:593:A:THR:H   | 15       | 0.24          |
| (1,1039) | 1:592:A:LEU:HD12 | 1:593:A:THR:H   | 15       | 0.24          |
| (1,1039) | 1:592:A:LEU:HD13 | 1:593:A:THR:H   | 15       | 0.24          |
| (1,1039) | 1:592:A:LEU:HD21 | 1:593:A:THR:H   | 15       | 0.24          |
| (1,1039) | 1:592:A:LEU:HD22 | 1:593:A:THR:H   | 15       | 0.24          |
| (1,1039) | 1:592:A:LEU:HD23 | 1:593:A:THR:H   | 15       | 0.24          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1 | 12       | 0.24          |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2 | 12       | 0.24          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1 | 12       | 0.24          |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2 | 12       | 0.24          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1 | 12       | 0.24          |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2 | 12       | 0.24          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD1 | 8        | 0.24          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD2 | 8        | 0.24          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD1 | 8        | 0.24          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD2 | 8        | 0.24          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD1 | 11       | 0.24          |
| (1,235)  | 1:544:A:LEU:HD11 | 1:652:A:PHE:HD2 | 11       | 0.24          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD1 | 11       | 0.24          |
| (1,235)  | 1:544:A:LEU:HD12 | 1:652:A:PHE:HD2 | 11       | 0.24          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD1 | 11       | 0.24          |
| (1,235)  | 1:544:A:LEU:HD13 | 1:652:A:PHE:HD2 | 11       | 0.24          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H   | 15       | 0.24          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H   | 15       | 0.24          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H   | 15       | 0.24          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H   | 15       | 0.24          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H   | 15       | 0.24          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H   | 15       | 0.24          |
| (1,1071) | 1:594:A:LYS:HB2  | 1:594:A:LYS:HD2 | 19       | 0.23          |
| (1,1071) | 1:594:A:LYS:HB2  | 1:594:A:LYS:HD3 | 19       | 0.23          |
| (1,1071) | 1:594:A:LYS:HB3  | 1:594:A:LYS:HD2 | 19       | 0.23          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1071) | 1:594:A:LYS:HB3  | 1:594:A:LYS:HD3  | 19       | 0.23          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 6        | 0.23          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 6        | 0.23          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 6        | 0.23          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 6        | 0.23          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 1        | 0.23          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 1        | 0.23          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 1        | 0.23          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 1        | 0.23          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 1        | 0.23          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 1        | 0.23          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1  | 14       | 0.23          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2  | 14       | 0.23          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1  | 14       | 0.23          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2  | 14       | 0.23          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1  | 14       | 0.23          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2  | 14       | 0.23          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H    | 8        | 0.23          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H    | 8        | 0.23          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H    | 8        | 0.23          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H    | 8        | 0.23          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H    | 8        | 0.23          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H    | 8        | 0.23          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 20       | 0.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 20       | 0.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 20       | 0.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 20       | 0.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 20       | 0.22          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 20       | 0.22          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG2  | 12       | 0.22          |
| (1,500)  | 1:562:A:PHE:HE1  | 1:629:A:ARG:HG3  | 12       | 0.22          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG2  | 12       | 0.22          |
| (1,500)  | 1:562:A:PHE:HE2  | 1:629:A:ARG:HG3  | 12       | 0.22          |
| (1,137)  | 1:538:A:LEU:HD11 | 1:584:A:ILE:H    | 9        | 0.22          |
| (1,137)  | 1:538:A:LEU:HD12 | 1:584:A:ILE:H    | 9        | 0.22          |
| (1,137)  | 1:538:A:LEU:HD13 | 1:584:A:ILE:H    | 9        | 0.22          |
| (1,137)  | 1:538:A:LEU:HD21 | 1:584:A:ILE:H    | 9        | 0.22          |
| (1,137)  | 1:538:A:LEU:HD22 | 1:584:A:ILE:H    | 9        | 0.22          |
| (1,137)  | 1:538:A:LEU:HD23 | 1:584:A:ILE:H    | 9        | 0.22          |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 18       | 0.21          |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 18       | 0.21          |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 18       | 0.21          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2 | 18       | 0.21          |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2 | 18       | 0.21          |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2 | 18       | 0.21          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD1 | 12       | 0.21          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD2 | 12       | 0.21          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD1 | 12       | 0.21          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD2 | 12       | 0.21          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD1 | 20       | 0.21          |
| (1,405)  | 1:556:A:MET:HE1  | 1:638:A:PHE:HD2 | 20       | 0.21          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD1 | 20       | 0.21          |
| (1,405)  | 1:556:A:MET:HE2  | 1:638:A:PHE:HD2 | 20       | 0.21          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD1 | 20       | 0.21          |
| (1,405)  | 1:556:A:MET:HE3  | 1:638:A:PHE:HD2 | 20       | 0.21          |
| (1,145)  | 1:538:A:LEU:HD11 | 1:605:A:SER:H   | 14       | 0.21          |
| (1,145)  | 1:538:A:LEU:HD12 | 1:605:A:SER:H   | 14       | 0.21          |
| (1,145)  | 1:538:A:LEU:HD13 | 1:605:A:SER:H   | 14       | 0.21          |
| (1,145)  | 1:538:A:LEU:HD21 | 1:605:A:SER:H   | 14       | 0.21          |
| (1,145)  | 1:538:A:LEU:HD22 | 1:605:A:SER:H   | 14       | 0.21          |
| (1,145)  | 1:538:A:LEU:HD23 | 1:605:A:SER:H   | 14       | 0.21          |
| (1,1429) | 1:643:A:GLU:HB2  | 1:643:A:GLU:HG2 | 1        | 0.2           |
| (1,1097) | 1:597:A:LYS:HB3  | 1:598:A:GLU:HA  | 19       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HB2 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HB3 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HB2 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HB3 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HB2 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HB3 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HB2 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HB3 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HB2 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HB3 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HB2 | 20       | 0.2           |
| (1,1042) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HB3 | 20       | 0.2           |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H   | 16       | 0.2           |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD1 | 3        | 0.2           |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD2 | 3        | 0.2           |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD1 | 3        | 0.2           |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD2 | 3        | 0.2           |
| (1,240)  | 1:544:A:LEU:HD21 | 1:652:A:PHE:HD1 | 3        | 0.2           |
| (1,240)  | 1:544:A:LEU:HD21 | 1:652:A:PHE:HD2 | 3        | 0.2           |
| (1,240)  | 1:544:A:LEU:HD22 | 1:652:A:PHE:HD1 | 3        | 0.2           |
| (1,240)  | 1:544:A:LEU:HD22 | 1:652:A:PHE:HD2 | 3        | 0.2           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,240)  | 1:544:A:LEU:HD23 | 1:652:A:PHE:HD1  | 3        | 0.2           |
| (1,240)  | 1:544:A:LEU:HD23 | 1:652:A:PHE:HD2  | 3        | 0.2           |
| (1,143)  | 1:538:A:LEU:HD11 | 1:604:A:GLY:H    | 11       | 0.2           |
| (1,143)  | 1:538:A:LEU:HD12 | 1:604:A:GLY:H    | 11       | 0.2           |
| (1,143)  | 1:538:A:LEU:HD13 | 1:604:A:GLY:H    | 11       | 0.2           |
| (1,143)  | 1:538:A:LEU:HD21 | 1:604:A:GLY:H    | 11       | 0.2           |
| (1,143)  | 1:538:A:LEU:HD22 | 1:604:A:GLY:H    | 11       | 0.2           |
| (1,143)  | 1:538:A:LEU:HD23 | 1:604:A:GLY:H    | 11       | 0.2           |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 1        | 0.19          |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 1        | 0.19          |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 1        | 0.19          |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 1        | 0.19          |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 1        | 0.19          |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 1        | 0.19          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD1  | 1        | 0.19          |
| (1,577)  | 1:566:A:GLN:HG2  | 1:627:A:TYR:HD2  | 1        | 0.19          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD1  | 1        | 0.19          |
| (1,577)  | 1:566:A:GLN:HG3  | 1:627:A:TYR:HD2  | 1        | 0.19          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 9        | 0.18          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 9        | 0.18          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 9        | 0.18          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 9        | 0.18          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 9        | 0.18          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 9        | 0.18          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 5        | 0.18          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 5        | 0.18          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 5        | 0.18          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 11       | 0.18          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 11       | 0.18          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 11       | 0.18          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 14       | 0.18          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 14       | 0.18          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 14       | 0.18          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 5        | 0.18          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 5        | 0.18          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 5        | 0.18          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 5        | 0.18          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 5        | 0.18          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 5        | 0.18          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 5        | 0.18          |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG2  | 8        | 0.18          |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG3  | 8        | 0.18          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG2  | 8        | 0.18          |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG3  | 8        | 0.18          |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG2  | 8        | 0.18          |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG3  | 8        | 0.18          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD11 | 14       | 0.18          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD12 | 14       | 0.18          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD13 | 14       | 0.18          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD21 | 14       | 0.18          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD22 | 14       | 0.18          |
| (1,127)  | 1:538:A:LEU:H    | 1:538:A:LEU:HD23 | 14       | 0.18          |
| (1,1327) | 1:635:A:VAL:HG21 | 1:636:A:ASP:HA   | 5        | 0.17          |
| (1,1327) | 1:635:A:VAL:HG22 | 1:636:A:ASP:HA   | 5        | 0.17          |
| (1,1327) | 1:635:A:VAL:HG23 | 1:636:A:ASP:HA   | 5        | 0.17          |
| (1,1185) | 1:611:A:CYS:HA   | 1:614:A:THR:H    | 20       | 0.17          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 1        | 0.17          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 1        | 0.17          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 1        | 0.17          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 7        | 0.17          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 7        | 0.17          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 7        | 0.17          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 12       | 0.17          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 12       | 0.17          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 12       | 0.17          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 6        | 0.17          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 6        | 0.17          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 6        | 0.17          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 6        | 0.17          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 6        | 0.17          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 6        | 0.17          |
| (1,729)  | 1:577:A:ILE:HB   | 1:577:A:ILE:HD11 | 16       | 0.17          |
| (1,729)  | 1:577:A:ILE:HB   | 1:577:A:ILE:HD12 | 16       | 0.17          |
| (1,729)  | 1:577:A:ILE:HB   | 1:577:A:ILE:HD13 | 16       | 0.17          |
| (1,139)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HA   | 11       | 0.17          |
| (1,139)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HA   | 11       | 0.17          |
| (1,139)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HA   | 11       | 0.17          |
| (1,139)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HA   | 11       | 0.17          |
| (1,139)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HA   | 11       | 0.17          |
| (1,139)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HA   | 11       | 0.17          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD11 | 11       | 0.16          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD12 | 11       | 0.16          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD13 | 11       | 0.16          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD21 | 11       | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD22 | 11       | 0.16          |
| (1,1592) | 1:660:A:LEU:HA   | 1:660:A:LEU:HD23 | 11       | 0.16          |
| (1,1585) | 1:657:A:ILE:HB   | 1:657:A:ILE:HD11 | 7        | 0.16          |
| (1,1585) | 1:657:A:ILE:HB   | 1:657:A:ILE:HD12 | 7        | 0.16          |
| (1,1585) | 1:657:A:ILE:HB   | 1:657:A:ILE:HD13 | 7        | 0.16          |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD2  | 9        | 0.16          |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD3  | 9        | 0.16          |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD2  | 9        | 0.16          |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD3  | 9        | 0.16          |
| (1,1383) | 1:640:A:GLU:H    | 1:640:A:GLU:HG2  | 16       | 0.16          |
| (1,1327) | 1:635:A:VAL:HG21 | 1:636:A:ASP:HA   | 6        | 0.16          |
| (1,1327) | 1:635:A:VAL:HG22 | 1:636:A:ASP:HA   | 6        | 0.16          |
| (1,1327) | 1:635:A:VAL:HG23 | 1:636:A:ASP:HA   | 6        | 0.16          |
| (1,1327) | 1:635:A:VAL:HG21 | 1:636:A:ASP:HA   | 17       | 0.16          |
| (1,1327) | 1:635:A:VAL:HG22 | 1:636:A:ASP:HA   | 17       | 0.16          |
| (1,1327) | 1:635:A:VAL:HG23 | 1:636:A:ASP:HA   | 17       | 0.16          |
| (1,1264) | 1:626:A:THR:H    | 1:628:A:CYS:HB2  | 16       | 0.16          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 4        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 4        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 4        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 6        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 6        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 6        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 9        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 9        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 9        | 0.16          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 13       | 0.16          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 13       | 0.16          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 13       | 0.16          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 17       | 0.16          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 17       | 0.16          |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 17       | 0.16          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD11 | 1        | 0.16          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD12 | 1        | 0.16          |
| (1,788)  | 1:582:A:TYR:HD1  | 1:630:A:LEU:HD13 | 1        | 0.16          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD11 | 1        | 0.16          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD12 | 1        | 0.16          |
| (1,788)  | 1:582:A:TYR:HD2  | 1:630:A:LEU:HD13 | 1        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD11 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD12 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD13 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD21 | 4        | 0.16          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD22 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD2  | 1:538:A:LEU:HD23 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD11 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD12 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD13 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD21 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD22 | 4        | 0.16          |
| (1,124)  | 1:537:A:LYS:HD3  | 1:538:A:LEU:HD23 | 4        | 0.16          |
| (1,1264) | 1:626:A:THR:H    | 1:628:A:CYS:HB2  | 1        | 0.15          |
| (1,1264) | 1:626:A:THR:H    | 1:628:A:CYS:HB2  | 10       | 0.15          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD2  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD2  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD2  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD2  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD2  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD2  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD11 | 1:623:A:ARG:HD3  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD12 | 1:623:A:ARG:HD3  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD13 | 1:623:A:ARG:HD3  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD21 | 1:623:A:ARG:HD3  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD22 | 1:623:A:ARG:HD3  | 7        | 0.15          |
| (1,1045) | 1:592:A:LEU:HD23 | 1:623:A:ARG:HD3  | 7        | 0.15          |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 16       | 0.15          |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 16       | 0.15          |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 16       | 0.15          |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 16       | 0.15          |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 16       | 0.15          |
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 16       | 0.15          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 2        | 0.15          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 2        | 0.15          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 2        | 0.15          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 16       | 0.15          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 16       | 0.15          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 16       | 0.15          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 17       | 0.15          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 17       | 0.15          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 17       | 0.15          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 2        | 0.15          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 2        | 0.15          |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 2        | 0.15          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 6        | 0.15          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 6        | 0.15          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 6        | 0.15          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 7        | 0.15          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 7        | 0.15          |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 7        | 0.15          |
| (1,1015) | 1:591:A:VAL:HG11 | 1:593:A:THR:H    | 17       | 0.15          |
| (1,1015) | 1:591:A:VAL:HG12 | 1:593:A:THR:H    | 17       | 0.15          |
| (1,1015) | 1:591:A:VAL:HG13 | 1:593:A:THR:H    | 17       | 0.15          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 1        | 0.15          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD11 | 3        | 0.15          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD12 | 3        | 0.15          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD13 | 3        | 0.15          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD21 | 3        | 0.15          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD22 | 3        | 0.15          |
| (1,439)  | 1:559:A:LYS:HE2  | 1:633:A:LEU:HD23 | 3        | 0.15          |
| (1,1427) | 1:643:A:GLU:H    | 1:643:A:GLU:HB2  | 9        | 0.14          |
| (1,1427) | 1:643:A:GLU:H    | 1:643:A:GLU:HB2  | 13       | 0.14          |
| (1,1327) | 1:635:A:VAL:HG21 | 1:636:A:ASP:HA   | 1        | 0.14          |
| (1,1327) | 1:635:A:VAL:HG22 | 1:636:A:ASP:HA   | 1        | 0.14          |
| (1,1327) | 1:635:A:VAL:HG23 | 1:636:A:ASP:HA   | 1        | 0.14          |
| (1,1327) | 1:635:A:VAL:HG21 | 1:636:A:ASP:HA   | 8        | 0.14          |
| (1,1327) | 1:635:A:VAL:HG22 | 1:636:A:ASP:HA   | 8        | 0.14          |
| (1,1327) | 1:635:A:VAL:HG23 | 1:636:A:ASP:HA   | 8        | 0.14          |
| (1,1327) | 1:635:A:VAL:HG21 | 1:636:A:ASP:HA   | 15       | 0.14          |
| (1,1327) | 1:635:A:VAL:HG22 | 1:636:A:ASP:HA   | 15       | 0.14          |
| (1,1327) | 1:635:A:VAL:HG23 | 1:636:A:ASP:HA   | 15       | 0.14          |
| (1,1264) | 1:626:A:THR:H    | 1:628:A:CYS:HB2  | 5        | 0.14          |
| (1,1044) | 1:592:A:LEU:HD11 | 1:623:A:ARG:H    | 4        | 0.14          |
| (1,1044) | 1:592:A:LEU:HD12 | 1:623:A:ARG:H    | 4        | 0.14          |
| (1,1044) | 1:592:A:LEU:HD13 | 1:623:A:ARG:H    | 4        | 0.14          |
| (1,1044) | 1:592:A:LEU:HD21 | 1:623:A:ARG:H    | 4        | 0.14          |
| (1,1044) | 1:592:A:LEU:HD22 | 1:623:A:ARG:H    | 4        | 0.14          |
| (1,1044) | 1:592:A:LEU:HD23 | 1:623:A:ARG:H    | 4        | 0.14          |
| (1,1022) | 1:591:A:VAL:HG21 | 1:600:A:LYS:HA   | 3        | 0.14          |
| (1,1022) | 1:591:A:VAL:HG22 | 1:600:A:LYS:HA   | 3        | 0.14          |
| (1,1022) | 1:591:A:VAL:HG23 | 1:600:A:LYS:HA   | 3        | 0.14          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 3        | 0.14          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 4        | 0.14          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 7        | 0.14          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 9        | 0.14          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 12       | 0.14          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 14       | 0.14          |
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD2  | 14       | 0.13          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1506) | 1:650:A:ARG:HB2  | 1:650:A:ARG:HD3  | 14       | 0.13          |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD2  | 14       | 0.13          |
| (1,1506) | 1:650:A:ARG:HB3  | 1:650:A:ARG:HD3  | 14       | 0.13          |
| (1,1264) | 1:626:A:THR:H    | 1:628:A:CYS:HB2  | 4        | 0.13          |
| (1,1264) | 1:626:A:THR:H    | 1:628:A:CYS:HB2  | 11       | 0.13          |
| (1,1127) | 1:600:A:LYS:HD3  | 1:601:A:LEU:H    | 13       | 0.13          |
| (1,1043) | 1:592:A:LEU:HD11 | 1:599:A:MET:H    | 19       | 0.13          |
| (1,1043) | 1:592:A:LEU:HD12 | 1:599:A:MET:H    | 19       | 0.13          |
| (1,1043) | 1:592:A:LEU:HD13 | 1:599:A:MET:H    | 19       | 0.13          |
| (1,1043) | 1:592:A:LEU:HD21 | 1:599:A:MET:H    | 19       | 0.13          |
| (1,1043) | 1:592:A:LEU:HD22 | 1:599:A:MET:H    | 19       | 0.13          |
| (1,1043) | 1:592:A:LEU:HD23 | 1:599:A:MET:H    | 19       | 0.13          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 5        | 0.13          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 5        | 0.13          |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 5        | 0.13          |
| (1,1015) | 1:591:A:VAL:HG11 | 1:593:A:THR:H    | 2        | 0.13          |
| (1,1015) | 1:591:A:VAL:HG12 | 1:593:A:THR:H    | 2        | 0.13          |
| (1,1015) | 1:591:A:VAL:HG13 | 1:593:A:THR:H    | 2        | 0.13          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 2        | 0.13          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 11       | 0.13          |
| (1,728)  | 1:577:A:ILE:HA   | 1:618:A:ARG:H    | 16       | 0.13          |
| (1,696)  | 1:574:A:GLU:HA   | 1:579:A:LYS:HD2  | 9        | 0.13          |
| (1,696)  | 1:574:A:GLU:HA   | 1:579:A:LYS:HD3  | 9        | 0.13          |
| (1,1619) | 1:663:A:ILE:HG21 | 1:663:A:ILE:HG13 | 1        | 0.12          |
| (1,1619) | 1:663:A:ILE:HG22 | 1:663:A:ILE:HG13 | 1        | 0.12          |
| (1,1619) | 1:663:A:ILE:HG23 | 1:663:A:ILE:HG13 | 1        | 0.12          |
| (1,1429) | 1:643:A:GLU:HB2  | 1:643:A:GLU:HG2  | 4        | 0.12          |
| (1,1264) | 1:626:A:THR:H    | 1:628:A:CYS:HB2  | 19       | 0.12          |
| (1,1015) | 1:591:A:VAL:HG11 | 1:593:A:THR:H    | 1        | 0.12          |
| (1,1015) | 1:591:A:VAL:HG12 | 1:593:A:THR:H    | 1        | 0.12          |
| (1,1015) | 1:591:A:VAL:HG13 | 1:593:A:THR:H    | 1        | 0.12          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 6        | 0.12          |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 17       | 0.12          |
| (1,743)  | 1:578:A:GLY:H    | 1:579:A:LYS:HA   | 16       | 0.12          |
| (1,653)  | 1:572:A:ILE:H    | 1:572:A:ILE:HG12 | 14       | 0.12          |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG2  | 9        | 0.12          |
| (1,205)  | 1:542:A:MET:HE1  | 1:543:A:PRO:HG3  | 9        | 0.12          |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG2  | 9        | 0.12          |
| (1,205)  | 1:542:A:MET:HE2  | 1:543:A:PRO:HG3  | 9        | 0.12          |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG2  | 9        | 0.12          |
| (1,205)  | 1:542:A:MET:HE3  | 1:543:A:PRO:HG3  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HG2  | 9        | 0.12          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,140)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HG2  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HG2  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HG2  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HG2  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HG2  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD11 | 1:585:A:GLN:HG3  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD12 | 1:585:A:GLN:HG3  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD13 | 1:585:A:GLN:HG3  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD21 | 1:585:A:GLN:HG3  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD22 | 1:585:A:GLN:HG3  | 9        | 0.12          |
| (1,140)  | 1:538:A:LEU:HD23 | 1:585:A:GLN:HG3  | 9        | 0.12          |
| (1,118)  | 1:537:A:LYS:HA   | 1:537:A:LYS:HD2  | 19       | 0.12          |
| (1,118)  | 1:537:A:LYS:HA   | 1:537:A:LYS:HD3  | 19       | 0.12          |
| (1,1588) | 1:659:A:ARG:H    | 1:659:A:ARG:HB2  | 1        | 0.11          |
| (1,1588) | 1:659:A:ARG:H    | 1:659:A:ARG:HB2  | 14       | 0.11          |
| (1,1427) | 1:643:A:GLU:H    | 1:643:A:GLU:HB2  | 14       | 0.11          |
| (1,1392) | 1:640:A:GLU:HB3  | 1:641:A:VAL:HG11 | 4        | 0.11          |
| (1,1392) | 1:640:A:GLU:HB3  | 1:641:A:VAL:HG12 | 4        | 0.11          |
| (1,1392) | 1:640:A:GLU:HB3  | 1:641:A:VAL:HG13 | 4        | 0.11          |
| (1,1317) | 1:635:A:VAL:H    | 1:636:A:ASP:HB2  | 4        | 0.11          |
| (1,1127) | 1:600:A:LYS:HD3  | 1:601:A:LEU:H    | 11       | 0.11          |
| (1,1127) | 1:600:A:LYS:HD3  | 1:601:A:LEU:H    | 17       | 0.11          |
| (1,1106) | 1:598:A:GLU:HG3  | 1:599:A:MET:H    | 3        | 0.11          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 2        | 0.11          |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 2        | 0.11          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 2        | 0.11          |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 2        | 0.11          |
| (1,1074) | 1:595:A:GLY:HA2  | 1:596:A:ASN:HB3  | 10       | 0.11          |
| (1,1074) | 1:595:A:GLY:HA3  | 1:596:A:ASN:HB3  | 10       | 0.11          |
| (1,1074) | 1:595:A:GLY:HA2  | 1:596:A:ASN:HB3  | 17       | 0.11          |
| (1,1074) | 1:595:A:GLY:HA3  | 1:596:A:ASN:HB3  | 17       | 0.11          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 1        | 0.11          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 1        | 0.11          |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 1        | 0.11          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 12       | 0.11          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 12       | 0.11          |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 12       | 0.11          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 14       | 0.11          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 14       | 0.11          |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 14       | 0.11          |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 16       | 0.11          |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 16       | 0.11          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 16       | 0.11          |
| (1,1015) | 1:591:A:VAL:HG11 | 1:593:A:THR:H    | 7        | 0.11          |
| (1,1015) | 1:591:A:VAL:HG12 | 1:593:A:THR:H    | 7        | 0.11          |
| (1,1015) | 1:591:A:VAL:HG13 | 1:593:A:THR:H    | 7        | 0.11          |
| (1,1015) | 1:591:A:VAL:HG11 | 1:593:A:THR:H    | 9        | 0.11          |
| (1,1015) | 1:591:A:VAL:HG12 | 1:593:A:THR:H    | 9        | 0.11          |
| (1,1015) | 1:591:A:VAL:HG13 | 1:593:A:THR:H    | 9        | 0.11          |
| (1,1014) | 1:591:A:VAL:HG11 | 1:592:A:LEU:HA   | 14       | 0.11          |
| (1,1014) | 1:591:A:VAL:HG12 | 1:592:A:LEU:HA   | 14       | 0.11          |
| (1,1014) | 1:591:A:VAL:HG13 | 1:592:A:LEU:HA   | 14       | 0.11          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD11 | 10       | 0.11          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD12 | 10       | 0.11          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD13 | 10       | 0.11          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD21 | 10       | 0.11          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD22 | 10       | 0.11          |
| (1,994)  | 1:590:A:SER:HB3  | 1:592:A:LEU:HD23 | 10       | 0.11          |
| (1,696)  | 1:574:A:GLU:HA   | 1:579:A:LYS:HD2  | 12       | 0.11          |
| (1,696)  | 1:574:A:GLU:HA   | 1:579:A:LYS:HD3  | 12       | 0.11          |
| (1,567)  | 1:566:A:GLN:HA   | 1:627:A:TYR:HB3  | 18       | 0.11          |
| (1,257)  | 1:546:A:ALA:H    | 1:547:A:ASN:HB3  | 3        | 0.11          |
| (1,1611) | 1:663:A:ILE:H    | 1:664:A:GLY:H    | 19       | 0.1           |
| (1,1219) | 1:613:A:LEU:HG   | 1:614:A:THR:H    | 19       | 0.1           |
| (1,1206) | 1:612:A:LEU:HD21 | 1:638:A:PHE:HA   | 16       | 0.1           |
| (1,1206) | 1:612:A:LEU:HD22 | 1:638:A:PHE:HA   | 16       | 0.1           |
| (1,1206) | 1:612:A:LEU:HD23 | 1:638:A:PHE:HA   | 16       | 0.1           |
| (1,1185) | 1:611:A:CYS:HA   | 1:614:A:THR:H    | 6        | 0.1           |
| (1,1127) | 1:600:A:LYS:HD3  | 1:601:A:LEU:H    | 1        | 0.1           |
| (1,1121) | 1:600:A:LYS:H    | 1:600:A:LYS:HG2  | 7        | 0.1           |
| (1,1121) | 1:600:A:LYS:H    | 1:600:A:LYS:HG3  | 7        | 0.1           |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE2  | 7        | 0.1           |
| (1,1100) | 1:597:A:LYS:HG2  | 1:597:A:LYS:HE3  | 7        | 0.1           |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE2  | 7        | 0.1           |
| (1,1100) | 1:597:A:LYS:HG3  | 1:597:A:LYS:HE3  | 7        | 0.1           |
| (1,1084) | 1:596:A:ASN:HB2  | 1:597:A:LYS:HE2  | 2        | 0.1           |
| (1,1084) | 1:596:A:ASN:HB2  | 1:597:A:LYS:HE3  | 2        | 0.1           |
| (1,1074) | 1:595:A:GLY:HA2  | 1:596:A:ASN:HB3  | 5        | 0.1           |
| (1,1074) | 1:595:A:GLY:HA3  | 1:596:A:ASN:HB3  | 5        | 0.1           |
| (1,1041) | 1:592:A:LEU:HD11 | 1:598:A:GLU:HG2  | 15       | 0.1           |
| (1,1041) | 1:592:A:LEU:HD12 | 1:598:A:GLU:HG2  | 15       | 0.1           |
| (1,1041) | 1:592:A:LEU:HD13 | 1:598:A:GLU:HG2  | 15       | 0.1           |
| (1,1041) | 1:592:A:LEU:HD21 | 1:598:A:GLU:HG2  | 15       | 0.1           |
| (1,1041) | 1:592:A:LEU:HD22 | 1:598:A:GLU:HG2  | 15       | 0.1           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1041) | 1:592:A:LEU:HD23 | 1:598:A:GLU:HG2  | 15       | 0.1           |
| (1,1019) | 1:591:A:VAL:HG21 | 1:599:A:MET:HA   | 3        | 0.1           |
| (1,1019) | 1:591:A:VAL:HG22 | 1:599:A:MET:HA   | 3        | 0.1           |
| (1,1019) | 1:591:A:VAL:HG23 | 1:599:A:MET:HA   | 3        | 0.1           |
| (1,1015) | 1:591:A:VAL:HG11 | 1:593:A:THR:H    | 6        | 0.1           |
| (1,1015) | 1:591:A:VAL:HG12 | 1:593:A:THR:H    | 6        | 0.1           |
| (1,1015) | 1:591:A:VAL:HG13 | 1:593:A:THR:H    | 6        | 0.1           |
| (1,986)  | 1:590:A:SER:HA   | 1:600:A:LYS:H    | 13       | 0.1           |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD1  | 20       | 0.1           |
| (1,842)  | 1:584:A:ILE:HD11 | 1:607:A:PHE:HD2  | 20       | 0.1           |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD1  | 20       | 0.1           |
| (1,842)  | 1:584:A:ILE:HD12 | 1:607:A:PHE:HD2  | 20       | 0.1           |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD1  | 20       | 0.1           |
| (1,842)  | 1:584:A:ILE:HD13 | 1:607:A:PHE:HD2  | 20       | 0.1           |
| (1,645)  | 1:571:A:ILE:HG21 | 1:572:A:ILE:HD11 | 9        | 0.1           |
| (1,645)  | 1:571:A:ILE:HG21 | 1:572:A:ILE:HD12 | 9        | 0.1           |
| (1,645)  | 1:571:A:ILE:HG21 | 1:572:A:ILE:HD13 | 9        | 0.1           |
| (1,645)  | 1:571:A:ILE:HG22 | 1:572:A:ILE:HD11 | 9        | 0.1           |
| (1,645)  | 1:571:A:ILE:HG22 | 1:572:A:ILE:HD12 | 9        | 0.1           |
| (1,645)  | 1:571:A:ILE:HG22 | 1:572:A:ILE:HD13 | 9        | 0.1           |
| (1,645)  | 1:571:A:ILE:HG23 | 1:572:A:ILE:HD11 | 9        | 0.1           |
| (1,645)  | 1:571:A:ILE:HG23 | 1:572:A:ILE:HD12 | 9        | 0.1           |
| (1,645)  | 1:571:A:ILE:HG23 | 1:572:A:ILE:HD13 | 9        | 0.1           |
| (1,595)  | 1:568:A:GLY:H    | 1:569:A:ASP:HA   | 3        | 0.1           |
| (1,595)  | 1:568:A:GLY:H    | 1:569:A:ASP:HA   | 10       | 0.1           |
| (1,567)  | 1:566:A:GLN:HA   | 1:627:A:TYR:HB3  | 1        | 0.1           |
| (1,519)  | 1:564:A:VAL:H    | 1:629:A:ARG:HA   | 16       | 0.1           |
| (1,257)  | 1:546:A:ALA:H    | 1:547:A:ASN:HB3  | 16       | 0.1           |
| (1,183)  | 1:542:A:MET:H    | 1:542:A:MET:HG2  | 7        | 0.1           |

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

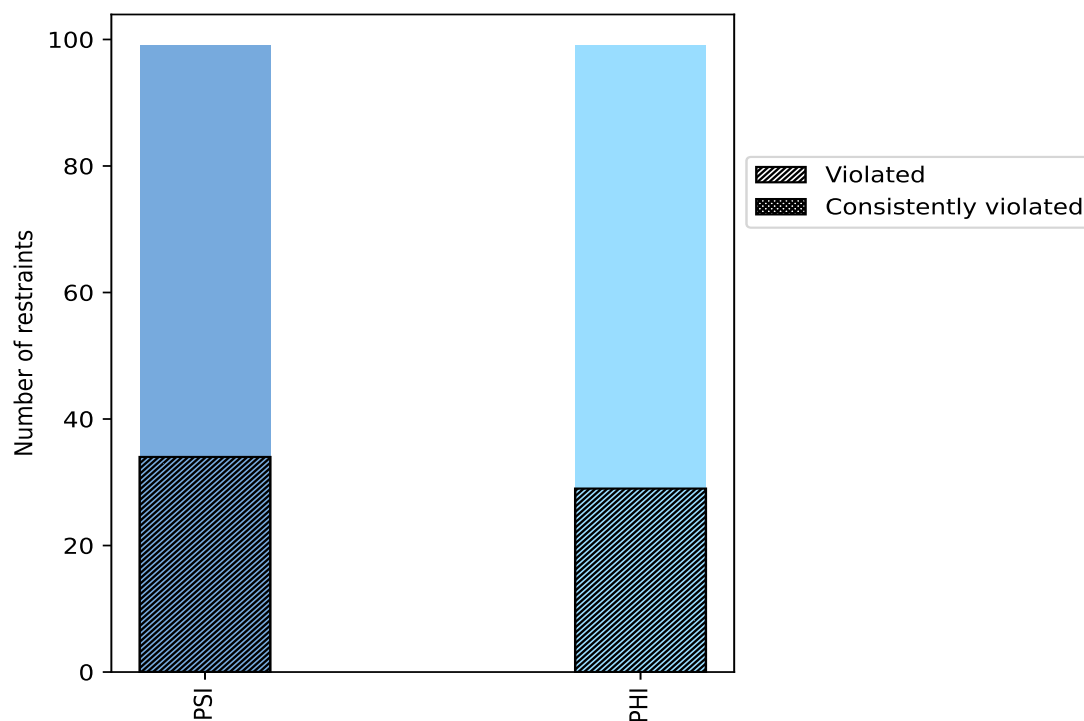
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 99    | 50.0           | 34                    | 34.3           | 17.2           | 0                                  | 0.0            | 0.0            |
| PHI        | 99    | 50.0           | 29                    | 29.3           | 14.6           | 0                                  | 0.0            | 0.0            |
| Total      | 198   | 100.0          | 63                    | 31.8           | 31.8           | 0                                  | 0.0            | 0.0            |

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

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



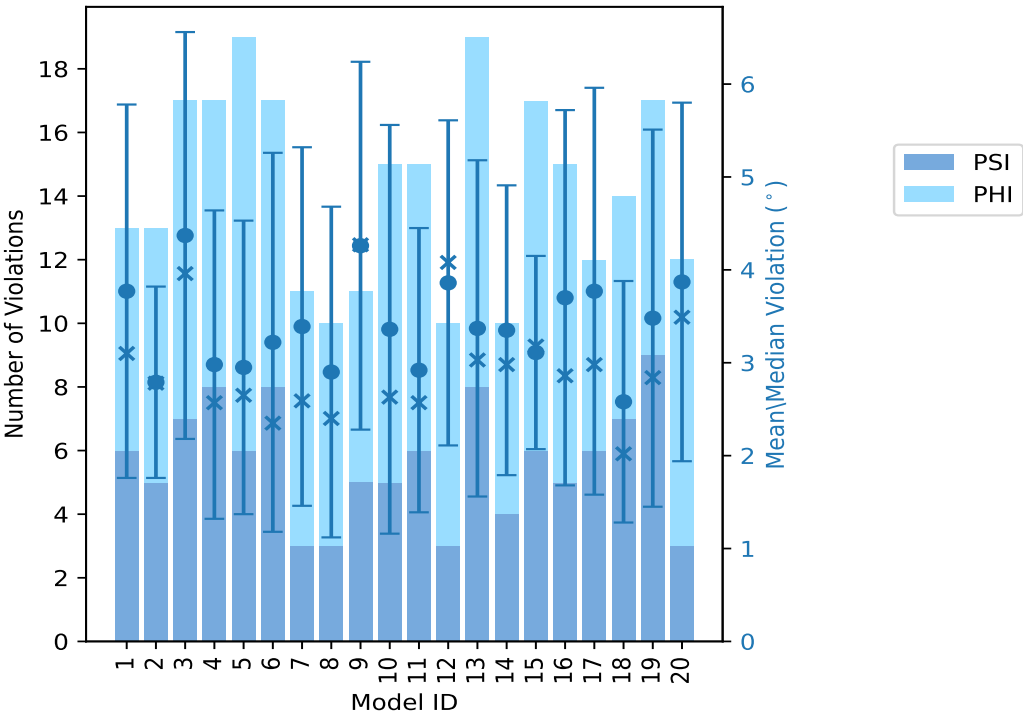
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 6                    | 7   | 13    | 3.77     | 7.53    | 2.01   | 3.1        |
| 2        | 5                    | 8   | 13    | 2.79     | 4.37    | 1.03   | 2.78       |
| 3        | 7                    | 10  | 17    | 4.37     | 8.89    | 2.19   | 3.96       |
| 4        | 8                    | 9   | 17    | 2.98     | 6.42    | 1.66   | 2.57       |
| 5        | 6                    | 13  | 19    | 2.95     | 6.58    | 1.58   | 2.65       |
| 6        | 8                    | 9   | 17    | 3.22     | 8.06    | 2.04   | 2.35       |
| 7        | 3                    | 8   | 11    | 3.39     | 8.21    | 1.93   | 2.59       |
| 8        | 3                    | 7   | 10    | 2.9      | 6.4     | 1.78   | 2.4        |
| 9        | 5                    | 6   | 11    | 4.26     | 8.35    | 1.98   | 4.27       |
| 10       | 5                    | 10  | 15    | 3.36     | 8.46    | 2.2    | 2.63       |
| 11       | 6                    | 9   | 15    | 2.92     | 5.9     | 1.53   | 2.57       |
| 12       | 3                    | 7   | 10    | 3.86     | 7.41    | 1.75   | 4.08       |
| 13       | 8                    | 11  | 19    | 3.37     | 7.36    | 1.81   | 3.03       |
| 14       | 4                    | 6   | 10    | 3.35     | 5.99    | 1.56   | 2.98       |
| 15       | 6                    | 11  | 17    | 3.11     | 4.89    | 1.04   | 3.18       |
| 16       | 5                    | 10  | 15    | 3.7      | 7.82    | 2.02   | 2.86       |
| 17       | 6                    | 6   | 12    | 3.77     | 7.87    | 2.19   | 2.98       |
| 18       | 7                    | 7   | 14    | 2.58     | 5.54    | 1.3    | 2.02       |
| 19       | 9                    | 8   | 17    | 3.48     | 7.81    | 2.03   | 2.84       |
| 20       | 3                    | 9   | 12    | 3.87     | 7.71    | 1.93   | 3.49       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

| Number of violated restraints |     |       | Fraction of the ensemble |      |
|-------------------------------|-----|-------|--------------------------|------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %    |
| 13                            | 7   | 20    | 1                        | 5.0  |
| 6                             | 4   | 10    | 2                        | 10.0 |
| 3                             | 4   | 7     | 3                        | 15.0 |
| 3                             | 2   | 5     | 4                        | 20.0 |
| 3                             | 1   | 4     | 5                        | 25.0 |
| 2                             | 1   | 3     | 6                        | 30.0 |
| 0                             | 1   | 1     | 7                        | 35.0 |
| 1                             | 1   | 2     | 8                        | 40.0 |
| 2                             | 1   | 3     | 9                        | 45.0 |
| 0                             | 2   | 2     | 10                       | 50.0 |
| 0                             | 0   | 0     | 11                       | 55.0 |

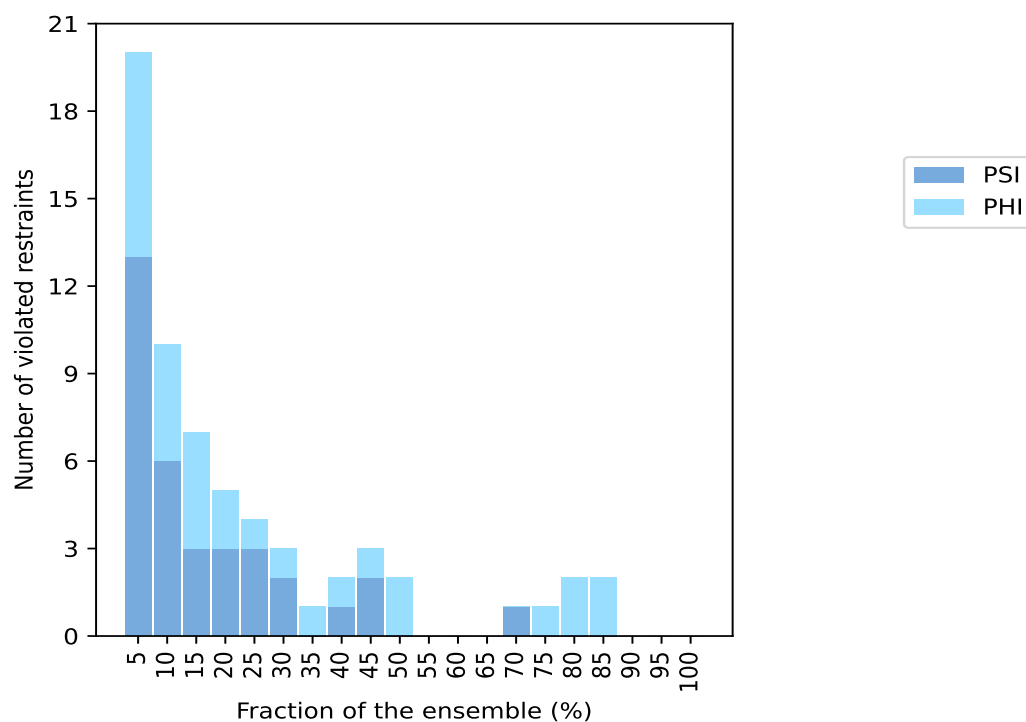
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| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 0                             | 0   | 0     | 12                       | 60.0  |
| 0                             | 0   | 0     | 13                       | 65.0  |
| 1                             | 0   | 1     | 14                       | 70.0  |
| 0                             | 1   | 1     | 15                       | 75.0  |
| 0                             | 2   | 2     | 16                       | 80.0  |
| 0                             | 2   | 2     | 17                       | 85.0  |
| 0                             | 0   | 0     | 18                       | 90.0  |
| 0                             | 0   | 0     | 19                       | 95.0  |
| 0                             | 0   | 0     | 20                       | 100.0 |

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

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

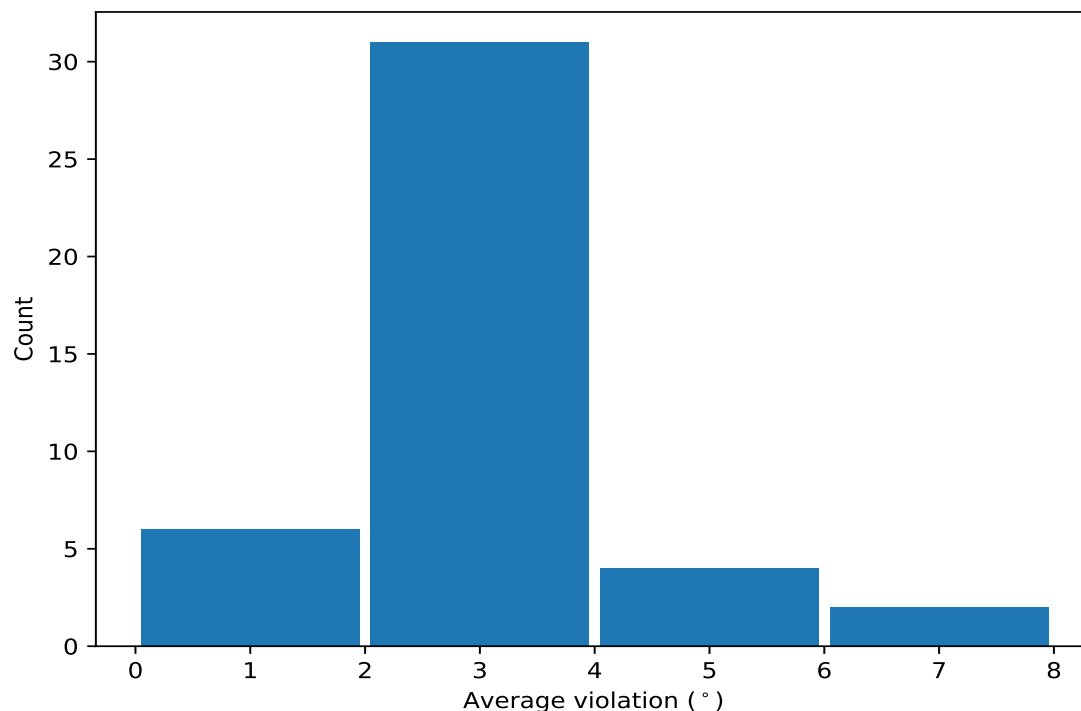


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 17                  | 3.83 | 1.83            | 3.75   |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 17                  | 3.44 | 1.46            | 3.1    |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 16                  | 4.84 | 1.63            | 4.98   |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 16                  | 3.77 | 1.74            | 3.53   |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 15                  | 2.81 | 1.41            | 2.43   |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 14                  | 6.04 | 1.59            | 6.02   |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 10                  | 2.54 | 0.96            | 2.51   |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 10                  | 2.28 | 1.18            | 1.92   |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 9                   | 3.85 | 1.27            | 3.85   |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 9                   | 2.35 | 1.05            | 2.09   |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 9                   | 1.85 | 0.69            | 1.54   |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 8                   | 4.27 | 2.12            | 3.65   |
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 8                   | 3.46 | 2.1             | 2.8    |
| (1,121) | 1:617:A:ARG:C | 1:618:A:ARG:N  | 1:618:A:ARG:CA | 1:618:A:ARG:C | 7                   | 3.57 | 1.97            | 3.03   |
| (1,198) | 1:662:A:ARG:N | 1:662:A:ARG:CA | 1:662:A:ARG:C  | 1:663:A:ILE:N | 6                   | 5.06 | 2.54            | 4.9    |
| (1,114) | 1:607:A:PHE:N | 1:607:A:PHE:CA | 1:607:A:PHE:C  | 1:608:A:GLY:N | 6                   | 3.73 | 2.0             | 3.1    |
| (1,75)  | 1:580:A:LYS:C | 1:581:A:MET:N  | 1:581:A:MET:CA | 1:581:A:MET:C | 6                   | 3.0  | 2.02            | 2.4    |
| (1,106) | 1:602:A:SER:N | 1:602:A:SER:CA | 1:602:A:SER:C  | 1:603:A:ASP:N | 5                   | 3.09 | 1.54            | 3.15   |
| (1,48)  | 1:561:A:LYS:N | 1:561:A:LYS:CA | 1:561:A:LYS:C  | 1:562:A:PHE:N | 5                   | 3.05 | 1.41            | 2.99   |
| (1,39)  | 1:556:A:MET:C | 1:557:A:LEU:N  | 1:557:A:LEU:CA | 1:557:A:LEU:C | 5                   | 2.41 | 1.15            | 1.91   |

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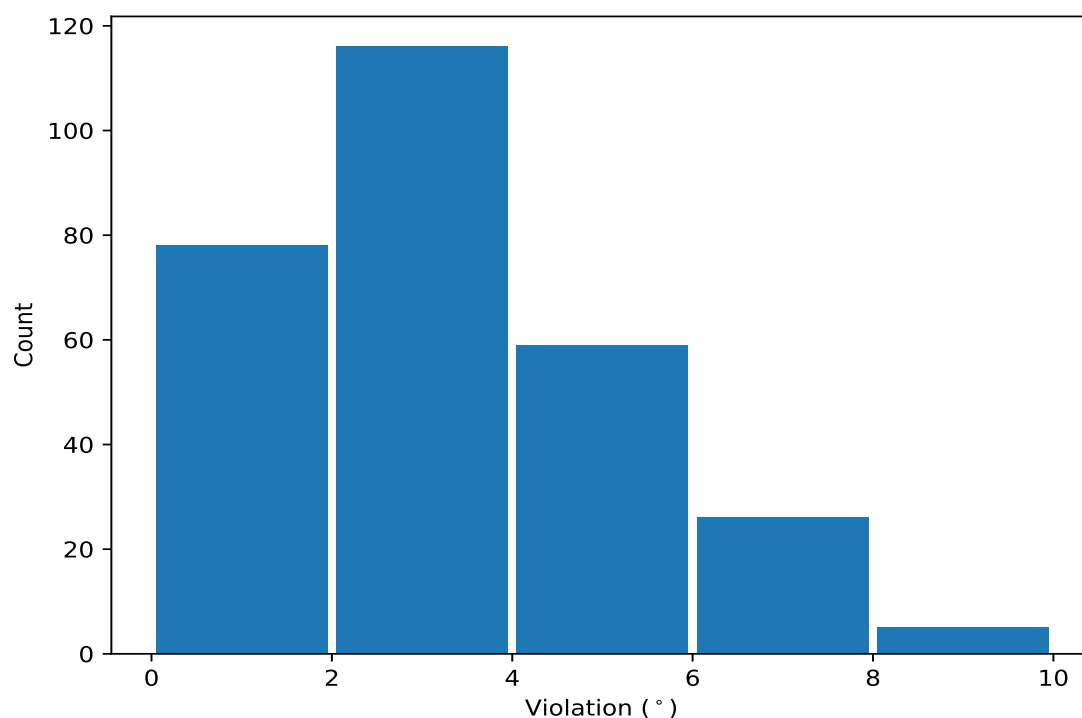
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,132) | 1:623:A:ARG:N | 1:623:A:ARG:CA | 1:623:A:ARG:C  | 1:624:A:ALA:N | 5                   | 2.01 | 0.33            | 1.89   |
| (1,63)  | 1:571:A:ILE:C | 1:572:A:ILE:N  | 1:572:A:ILE:CA | 1:572:A:ILE:C | 4                   | 3.2  | 0.87            | 2.76   |
| (1,128) | 1:621:A:SER:N | 1:621:A:SER:CA | 1:621:A:SER:C  | 1:622:A:VAL:N | 4                   | 1.98 | 0.64            | 2.02   |
| (1,195) | 1:659:A:ARG:C | 1:660:A:LEU:N  | 1:660:A:LEU:CA | 1:660:A:LEU:C | 4                   | 1.96 | 0.66            | 1.84   |
| (1,140) | 1:627:A:TYR:N | 1:627:A:TYR:CA | 1:627:A:TYR:C  | 1:628:A:CYS:N | 4                   | 1.95 | 0.58            | 1.86   |
| (1,160) | 1:637:A:ASN:N | 1:637:A:ASN:CA | 1:637:A:ASN:C  | 1:638:A:PHE:N | 4                   | 1.86 | 0.28            | 1.78   |
| (1,66)  | 1:573:A:ARG:N | 1:573:A:ARG:CA | 1:573:A:ARG:C  | 1:574:A:GLU:N | 3                   | 6.06 | 0.42            | 6.08   |
| (1,3)   | 1:536:A:ARG:C | 1:537:A:LYS:N  | 1:537:A:LYS:CA | 1:537:A:LYS:C | 3                   | 3.85 | 1.94            | 3.45   |
| (1,138) | 1:626:A:THR:N | 1:626:A:THR:CA | 1:626:A:THR:C  | 1:627:A:TYR:N | 3                   | 2.86 | 1.27            | 3.27   |
| (1,44)  | 1:559:A:LYS:N | 1:559:A:LYS:CA | 1:559:A:LYS:C  | 1:560:A:LEU:N | 3                   | 2.86 | 0.91            | 2.89   |
| (1,197) | 1:661:A:ASP:C | 1:662:A:ARG:N  | 1:662:A:ARG:CA | 1:662:A:ARG:C | 3                   | 2.85 | 1.64            | 2.12   |
| (1,21)  | 1:546:A:ALA:C | 1:547:A:ASN:N  | 1:547:A:ASN:CA | 1:547:A:ASN:C | 3                   | 2.45 | 1.66            | 1.55   |
| (1,147) | 1:630:A:LEU:C | 1:631:A:TYR:N  | 1:631:A:TYR:CA | 1:631:A:TYR:C | 3                   | 2.15 | 0.84            | 2.34   |
| (1,153) | 1:633:A:LEU:C | 1:634:A:SER:N  | 1:634:A:SER:CA | 1:634:A:SER:C | 2                   | 5.4  | 2.47            | 5.4    |
| (1,118) | 1:614:A:THR:N | 1:614:A:THR:CA | 1:614:A:THR:C  | 1:615:A:ARG:N | 2                   | 3.77 | 1.29            | 3.77   |
| (1,120) | 1:615:A:ARG:N | 1:615:A:ARG:CA | 1:615:A:ARG:C  | 1:616:A:GLY:N | 2                   | 3.43 | 0.23            | 3.43   |
| (1,68)  | 1:574:A:GLU:N | 1:574:A:GLU:CA | 1:574:A:GLU:C  | 1:575:A:GLY:N | 2                   | 2.8  | 0.75            | 2.8    |
| (1,115) | 1:612:A:LEU:C | 1:613:A:LEU:N  | 1:613:A:LEU:CA | 1:613:A:LEU:C | 2                   | 2.62 | 1.17            | 2.62   |
| (1,74)  | 1:580:A:LYS:N | 1:580:A:LYS:CA | 1:580:A:LYS:C  | 1:581:A:MET:N | 2                   | 2.58 | 1.18            | 2.58   |
| (1,109) | 1:604:A:GLY:C | 1:605:A:SER:N  | 1:605:A:SER:CA | 1:605:A:SER:C | 2                   | 2.49 | 0.01            | 2.49   |
| (1,165) | 1:639:A:ASN:C | 1:640:A:GLU:N  | 1:640:A:GLU:CA | 1:640:A:GLU:C | 2                   | 2.33 | 1.2             | 2.33   |
| (1,172) | 1:643:A:GLU:N | 1:643:A:GLU:CA | 1:643:A:GLU:C  | 1:644:A:GLU:N | 2                   | 2.16 | 0.86            | 2.16   |
| (1,192) | 1:655:A:VAL:N | 1:655:A:VAL:CA | 1:655:A:VAL:C  | 1:656:A:ALA:N | 2                   | 1.46 | 0.22            | 1.46   |

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

## 10.5 All violated dihedral-angle restraints ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 3        | 8.89          |
| (1,198) | 1:662:A:ARG:N | 1:662:A:ARG:CA | 1:662:A:ARG:C  | 1:663:A:ILE:N | 10       | 8.46          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 9        | 8.35          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 7        | 8.21          |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 6        | 8.06          |
| (1,153) | 1:633:A:LEU:C | 1:634:A:SER:N  | 1:634:A:SER:CA | 1:634:A:SER:C | 17       | 7.87          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 16       | 7.82          |
| (1,198) | 1:662:A:ARG:N | 1:662:A:ARG:CA | 1:662:A:ARG:C  | 1:663:A:ILE:N | 19       | 7.81          |
| (1,121) | 1:617:A:ARG:C | 1:618:A:ARG:N  | 1:618:A:ARG:CA | 1:618:A:ARG:C | 20       | 7.71          |
| (1,196) | 1:660:A:LEU:N | 1:660:A:LEU:CA | 1:660:A:LEU:C  | 1:661:A:ASP:N | 10       | 7.67          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 1        | 7.53          |
| (1,114) | 1:607:A:PHE:N | 1:607:A:PHE:CA | 1:607:A:PHE:C  | 1:608:A:GLY:N | 3        | 7.5           |
| (1,75)  | 1:580:A:LYS:C | 1:581:A:MET:N  | 1:581:A:MET:CA | 1:581:A:MET:C | 3        | 7.42          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 12       | 7.41          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 13       | 7.36          |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 1        | 7.24          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 16       | 7.22          |
| (1,159) | 1:636:A:ASP:C | 1:637:A:ASN:N  | 1:637:A:ASN:CA | 1:637:A:ASN:C | 3        | 7.2           |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 6        | 7.18          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 13       | 7.09          |
| (1,150) | 1:632:A:SER:N | 1:632:A:SER:CA | 1:632:A:SER:C  | 1:633:A:LEU:N | 17       | 7.01          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 5        | 6.58          |
| (1,66)  | 1:573:A:ARG:N | 1:573:A:ARG:CA | 1:573:A:ARG:C  | 1:574:A:GLU:N | 16       | 6.57          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 4        | 6.42          |
| (1,3)   | 1:536:A:ARG:C | 1:537:A:LYS:N  | 1:537:A:LYS:CA | 1:537:A:LYS:C | 8        | 6.4           |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 4        | 6.38          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 9        | 6.17          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 1        | 6.15          |
| (1,66)  | 1:573:A:ARG:N | 1:573:A:ARG:CA | 1:573:A:ARG:C  | 1:574:A:GLU:N | 9        | 6.08          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 19       | 6.08          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 19       | 6.06          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 14       | 5.99          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 19       | 5.91          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 11       | 5.9           |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 20       | 5.77          |
| (1,106) | 1:602:A:SER:N | 1:602:A:SER:CA | 1:602:A:SER:C  | 1:603:A:ASP:N | 6        | 5.74          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 17       | 5.73          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 17       | 5.69          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 14       | 5.67          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 11       | 5.67          |
| (1,66)  | 1:573:A:ARG:N | 1:573:A:ARG:CA | 1:573:A:ARG:C  | 1:574:A:GLU:N | 18       | 5.54          |
| (1,48)  | 1:561:A:LYS:N | 1:561:A:LYS:CA | 1:561:A:LYS:C  | 1:562:A:PHE:N | 20       | 5.53          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 4        | 5.52          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 16       | 5.45          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 5        | 5.42          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 19       | 5.4           |
| (1,198) | 1:662:A:ARG:N | 1:662:A:ARG:CA | 1:662:A:ARG:C  | 1:663:A:ILE:N | 1        | 5.32          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 3        | 5.25          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 20       | 5.24          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 12       | 5.23          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 13       | 5.21          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 11       | 5.2           |
| (1,197) | 1:661:A:ASP:C | 1:662:A:ARG:N  | 1:662:A:ARG:CA | 1:662:A:ARG:C | 13       | 5.12          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 5        | 5.12          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 8        | 5.1           |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 9        | 5.08          |
| (1,118) | 1:614:A:THR:N | 1:614:A:THR:CA | 1:614:A:THR:C  | 1:615:A:ARG:N | 10       | 5.06          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 20       | 5.05          |
| (1,186) | 1:652:A:PHE:N | 1:652:A:PHE:CA | 1:652:A:PHE:C  | 1:653:A:GLU:N | 18       | 5.01          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 12       | 5.01          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 13       | 4.95          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 15       | 4.89          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 9        | 4.85          |
| (1,78)  | 1:582:A:TYR:N | 1:582:A:TYR:CA | 1:582:A:TYR:C  | 1:583:A:PHE:N | 3        | 4.84          |
| (1,114) | 1:607:A:PHE:N | 1:607:A:PHE:CA | 1:607:A:PHE:C  | 1:608:A:GLY:N | 7        | 4.83          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 6        | 4.82          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 14       | 4.8           |
| (1,21)  | 1:546:A:ALA:C | 1:547:A:ASN:N  | 1:547:A:ASN:CA | 1:547:A:ASN:C | 15       | 4.78          |
| (1,121) | 1:617:A:ARG:C | 1:618:A:ARG:N  | 1:618:A:ARG:CA | 1:618:A:ARG:C | 5        | 4.71          |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 3        | 4.7           |
| (1,63)  | 1:571:A:ILE:C | 1:572:A:ILE:N  | 1:572:A:ILE:CA | 1:572:A:ILE:C | 12       | 4.7           |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 10       | 4.69          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 7        | 4.56          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 7        | 4.52          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 13       | 4.52          |
| (1,198) | 1:662:A:ARG:N | 1:662:A:ARG:CA | 1:662:A:ARG:C  | 1:663:A:ILE:N | 5        | 4.49          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 12       | 4.38          |
| (1,39)  | 1:556:A:MET:C | 1:557:A:LEU:N  | 1:557:A:LEU:CA | 1:557:A:LEU:C | 2        | 4.37          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 9        | 4.27          |
| (1,94)  | 1:593:A:THR:N | 1:593:A:THR:CA | 1:593:A:THR:C  | 1:594:A:LYS:N | 19       | 4.26          |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 16       | 4.22          |
| (1,138) | 1:626:A:THR:N | 1:626:A:THR:CA | 1:626:A:THR:C  | 1:627:A:TYR:N | 11       | 4.18          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 6        | 4.16          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 2        | 4.12          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 8        | 4.11          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 17       | 4.1           |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 2        | 4.06          |
| (1,110) | 1:605:A:SER:N | 1:605:A:SER:CA | 1:605:A:SER:C  | 1:606:A:TYR:N | 4        | 4.04          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 3        | 4.02          |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 15       | 4.01          |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 18       | 3.96          |
| (1,44)  | 1:559:A:LYS:N | 1:559:A:LYS:CA | 1:559:A:LYS:C  | 1:560:A:LEU:N | 19       | 3.96          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 3        | 3.96          |
| (1,167) | 1:640:A:GLU:C | 1:641:A:VAL:N  | 1:641:A:VAL:CA | 1:641:A:VAL:C | 15       | 3.88          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 2        | 3.85          |
| (1,114) | 1:607:A:PHE:N | 1:607:A:PHE:CA | 1:607:A:PHE:C  | 1:608:A:GLY:N | 20       | 3.83          |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 15       | 3.8           |
| (1,115) | 1:612:A:LEU:C | 1:613:A:LEU:N  | 1:613:A:LEU:CA | 1:613:A:LEU:C | 15       | 3.79          |
| (1,74)  | 1:580:A:LYS:N | 1:580:A:LYS:CA | 1:580:A:LYS:C  | 1:581:A:MET:N | 12       | 3.77          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 3        | 3.75          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 3        | 3.74          |
| (1,120) | 1:615:A:ARG:N | 1:615:A:ARG:CA | 1:615:A:ARG:C  | 1:616:A:GLY:N | 5        | 3.66          |
| (1,68)  | 1:574:A:GLU:N | 1:574:A:GLU:CA | 1:574:A:GLU:C  | 1:575:A:GLY:N | 8        | 3.54          |
| (1,165) | 1:639:A:ASN:C | 1:640:A:GLU:N  | 1:640:A:GLU:CA | 1:640:A:GLU:C | 10       | 3.53          |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 4        | 3.5           |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 6        | 3.47          |
| (1,121) | 1:617:A:ARG:C | 1:618:A:ARG:N  | 1:618:A:ARG:CA | 1:618:A:ARG:C | 10       | 3.46          |
| (1,3)   | 1:536:A:ARG:C | 1:537:A:LYS:N  | 1:537:A:LYS:CA | 1:537:A:LYS:C | 15       | 3.45          |
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 14       | 3.44          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 1        | 3.32          |
| (1,106) | 1:602:A:SER:N | 1:602:A:SER:CA | 1:602:A:SER:C  | 1:603:A:ASP:N | 13       | 3.31          |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 16       | 3.31          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 14       | 3.3           |
| (1,48)  | 1:561:A:LYS:N | 1:561:A:LYS:CA | 1:561:A:LYS:C  | 1:562:A:PHE:N | 13       | 3.3           |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 8        | 3.28          |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 6        | 3.28          |
| (1,138) | 1:626:A:THR:N | 1:626:A:THR:CA | 1:626:A:THR:C  | 1:627:A:TYR:N | 4        | 3.27          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 15       | 3.26          |
| (1,46)  | 1:560:A:LEU:N | 1:560:A:LEU:CA | 1:560:A:LEU:C  | 1:561:A:LYS:N | 19       | 3.22          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 1        | 3.22          |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 10       | 3.21          |
| (1,120) | 1:615:A:ARG:N | 1:615:A:ARG:CA | 1:615:A:ARG:C  | 1:616:A:GLY:N | 2        | 3.2           |
| (1,198) | 1:662:A:ARG:N | 1:662:A:ARG:CA | 1:662:A:ARG:C  | 1:663:A:ILE:N | 15       | 3.18          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 9        | 3.18          |
| (1,106) | 1:602:A:SER:N | 1:602:A:SER:CA | 1:602:A:SER:C  | 1:603:A:ASP:N | 20       | 3.15          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 1        | 3.1           |
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 1        | 3.1           |
| (1,147) | 1:630:A:LEU:C | 1:631:A:TYR:N  | 1:631:A:TYR:CA | 1:631:A:TYR:C | 17       | 3.07          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 15       | 3.07          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 13       | 3.05          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 7        | 3.04          |
| (1,121) | 1:617:A:ARG:C | 1:618:A:ARG:N  | 1:618:A:ARG:CA | 1:618:A:ARG:C | 13       | 3.03          |
| (1,172) | 1:643:A:GLU:N | 1:643:A:GLU:CA | 1:643:A:GLU:C  | 1:644:A:GLU:N | 16       | 3.02          |
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 15       | 3.02          |
| (1,64)  | 1:572:A:ILE:N | 1:572:A:ILE:CA | 1:572:A:ILE:C  | 1:573:A:ARG:N | 15       | 2.99          |
| (1,48)  | 1:561:A:LYS:N | 1:561:A:LYS:CA | 1:561:A:LYS:C  | 1:562:A:PHE:N | 11       | 2.99          |
| (1,39)  | 1:556:A:MET:C | 1:557:A:LEU:N  | 1:557:A:LEU:CA | 1:557:A:LEU:C | 3        | 2.98          |
| (1,153) | 1:633:A:LEU:C | 1:634:A:SER:N  | 1:634:A:SER:CA | 1:634:A:SER:C | 5        | 2.94          |
| (1,195) | 1:659:A:ARG:C | 1:660:A:LEU:N  | 1:660:A:LEU:CA | 1:660:A:LEU:C | 3        | 2.93          |
| (1,155) | 1:634:A:SER:C | 1:635:A:VAL:N  | 1:635:A:VAL:CA | 1:635:A:VAL:C | 4        | 2.92          |
| (1,121) | 1:617:A:ARG:C | 1:618:A:ARG:N  | 1:618:A:ARG:CA | 1:618:A:ARG:C | 2        | 2.89          |
| (1,44)  | 1:559:A:LYS:N | 1:559:A:LYS:CA | 1:559:A:LYS:C  | 1:560:A:LEU:N | 17       | 2.89          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 20       | 2.87          |
| (1,63)  | 1:571:A:ILE:C | 1:572:A:ILE:N  | 1:572:A:ILE:CA | 1:572:A:ILE:C | 16       | 2.86          |
| (1,140) | 1:627:A:TYR:N | 1:627:A:TYR:CA | 1:627:A:TYR:C  | 1:628:A:CYS:N | 19       | 2.84          |
| (1,128) | 1:621:A:SER:N | 1:621:A:SER:CA | 1:621:A:SER:C  | 1:622:A:VAL:N | 16       | 2.82          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 13       | 2.81          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 2        | 2.78          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 5        | 2.77          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 18       | 2.76          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 9        | 2.74          |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 5        | 2.74          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 4        | 2.7           |
| (1,63)  | 1:571:A:ILE:C | 1:572:A:ILE:N  | 1:572:A:ILE:CA | 1:572:A:ILE:C | 3        | 2.67          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 14       | 2.66          |
| (1,132) | 1:623:A:ARG:N | 1:623:A:ARG:CA | 1:623:A:ARG:C  | 1:624:A:ALA:N | 17       | 2.66          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 12       | 2.65          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 5        | 2.65          |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 18       | 2.65          |
| (1,75)  | 1:580:A:LYS:C | 1:581:A:MET:N  | 1:581:A:MET:CA | 1:581:A:MET:C | 20       | 2.64          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 10       | 2.63          |
| (1,123) | 1:618:A:ARG:C | 1:619:A:THR:N  | 1:619:A:THR:CA | 1:619:A:THR:C | 5        | 2.63          |
| (1,100) | 1:599:A:MET:N | 1:599:A:MET:CA | 1:599:A:MET:C  | 1:600:A:LYS:N | 16       | 2.61          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 11       | 2.6           |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 19       | 2.6           |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 7        | 2.59          |
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 11       | 2.59          |
| (1,63)  | 1:571:A:ILE:C | 1:572:A:ILE:N  | 1:572:A:ILE:CA | 1:572:A:ILE:C | 13       | 2.59          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 4        | 2.57          |
| (1,4)   | 1:537:A:LYS:N | 1:537:A:LYS:CA | 1:537:A:LYS:C  | 1:538:A:LEU:N | 11       | 2.57          |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 1        | 2.53          |
| (1,109) | 1:604:A:GLY:C | 1:605:A:SER:N  | 1:605:A:SER:CA | 1:605:A:SER:C | 16       | 2.5           |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 9        | 2.5           |
| (1,125) | 1:619:A:THR:C | 1:620:A:ALA:N  | 1:620:A:ALA:CA | 1:620:A:ALA:C | 14       | 2.48          |

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*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,118) | 1:614:A:THR:N | 1:614:A:THR:CA | 1:614:A:THR:C  | 1:615:A:ARG:N | 13       | 2.48          |
| (1,109) | 1:604:A:GLY:C | 1:605:A:SER:N  | 1:605:A:SER:CA | 1:605:A:SER:C | 7        | 2.48          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 6        | 2.48          |
| (1,75)  | 1:580:A:LYS:C | 1:581:A:MET:N  | 1:581:A:MET:CA | 1:581:A:MET:C | 18       | 2.44          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 10       | 2.43          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 1        | 2.42          |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 10       | 2.42          |
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 4        | 2.41          |
| (1,114) | 1:607:A:PHE:N | 1:607:A:PHE:CA | 1:607:A:PHE:C  | 1:608:A:GLY:N | 2        | 2.38          |
| (1,114) | 1:607:A:PHE:N | 1:607:A:PHE:CA | 1:607:A:PHE:C  | 1:608:A:GLY:N | 6        | 2.35          |
| (1,75)  | 1:580:A:LYS:C | 1:581:A:MET:N  | 1:581:A:MET:CA | 1:581:A:MET:C | 1        | 2.35          |
| (1,147) | 1:630:A:LEU:C | 1:631:A:TYR:N  | 1:631:A:TYR:CA | 1:631:A:TYR:C | 19       | 2.34          |
| (1,160) | 1:637:A:ASN:N | 1:637:A:ASN:CA | 1:637:A:ASN:C  | 1:638:A:PHE:N | 15       | 2.32          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 20       | 2.31          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 7        | 2.31          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 11       | 2.24          |
| (1,128) | 1:621:A:SER:N | 1:621:A:SER:CA | 1:621:A:SER:C  | 1:622:A:VAL:N | 2        | 2.24          |
| (1,43)  | 1:558:A:THR:C | 1:559:A:LYS:N  | 1:559:A:LYS:CA | 1:559:A:LYS:C | 11       | 2.22          |
| (1,195) | 1:659:A:ARG:C | 1:660:A:LEU:N  | 1:660:A:LEU:CA | 1:660:A:LEU:C | 16       | 2.21          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 5        | 2.14          |
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 6        | 2.14          |
| (1,197) | 1:661:A:ASP:C | 1:662:A:ARG:N  | 1:662:A:ARG:CA | 1:662:A:ARG:C | 4        | 2.12          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 7        | 2.11          |
| (1,67)  | 1:573:A:ARG:C | 1:574:A:GLU:N  | 1:574:A:GLU:CA | 1:574:A:GLU:C | 10       | 2.1           |
| (1,48)  | 1:561:A:LYS:N | 1:561:A:LYS:CA | 1:561:A:LYS:C  | 1:562:A:PHE:N | 6        | 2.1           |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 11       | 2.09          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 2        | 2.08          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 5        | 2.07          |
| (1,106) | 1:602:A:SER:N | 1:602:A:SER:CA | 1:602:A:SER:C  | 1:603:A:ASP:N | 18       | 2.06          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 15       | 2.05          |
| (1,68)  | 1:574:A:GLU:N | 1:574:A:GLU:CA | 1:574:A:GLU:C  | 1:575:A:GLY:N | 14       | 2.05          |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 14       | 2.05          |
| (1,140) | 1:627:A:TYR:N | 1:627:A:TYR:CA | 1:627:A:TYR:C  | 1:628:A:CYS:N | 4        | 1.99          |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 6        | 1.99          |
| (1,121) | 1:617:A:ARG:C | 1:618:A:ARG:N  | 1:618:A:ARG:CA | 1:618:A:ARG:C | 18       | 1.97          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 12       | 1.96          |
| (1,132) | 1:623:A:ARG:N | 1:623:A:ARG:CA | 1:623:A:ARG:C  | 1:624:A:ALA:N | 18       | 1.96          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 16       | 1.94          |
| (1,39)  | 1:556:A:MET:C | 1:557:A:LEU:N  | 1:557:A:LEU:CA | 1:557:A:LEU:C | 15       | 1.91          |
| (1,132) | 1:623:A:ARG:N | 1:623:A:ARG:CA | 1:623:A:ARG:C  | 1:624:A:ALA:N | 9        | 1.89          |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 18       | 1.89          |
| (1,5)   | 1:537:A:LYS:C | 1:538:A:LEU:N  | 1:538:A:LEU:CA | 1:538:A:LEU:C | 18       | 1.87          |
| (1,132) | 1:623:A:ARG:N | 1:623:A:ARG:CA | 1:623:A:ARG:C  | 1:624:A:ALA:N | 3        | 1.82          |
| (1,73)  | 1:579:A:LYS:C | 1:580:A:LYS:N  | 1:580:A:LYS:CA | 1:580:A:LYS:C | 5        | 1.82          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 11       | 1.81          |
| (1,160) | 1:637:A:ASN:N | 1:637:A:ASN:CA | 1:637:A:ASN:C  | 1:638:A:PHE:N | 17       | 1.81          |
| (1,128) | 1:621:A:SER:N | 1:621:A:SER:CA | 1:621:A:SER:C  | 1:622:A:VAL:N | 9        | 1.79          |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 12       | 1.79          |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 17       | 1.79          |
| (1,75)  | 1:580:A:LYS:C | 1:581:A:MET:N  | 1:581:A:MET:CA | 1:581:A:MET:C | 19       | 1.78          |
| (1,50)  | 1:562:A:PHE:N | 1:562:A:PHE:CA | 1:562:A:PHE:C  | 1:563:A:GLU:N | 18       | 1.77          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,160) | 1:637:A:ASN:N | 1:637:A:ASN:CA | 1:637:A:ASN:C  | 1:638:A:PHE:N | 19       | 1.76          |
| (1,140) | 1:627:A:TYR:N | 1:627:A:TYR:CA | 1:627:A:TYR:C  | 1:628:A:CYS:N | 13       | 1.74          |
| (1,132) | 1:623:A:ARG:N | 1:623:A:ARG:CA | 1:623:A:ARG:C  | 1:624:A:ALA:N | 12       | 1.74          |
| (1,44)  | 1:559:A:LYS:N | 1:559:A:LYS:CA | 1:559:A:LYS:C  | 1:560:A:LEU:N | 13       | 1.72          |
| (1,193) | 1:658:A:ASP:C | 1:659:A:ARG:N  | 1:659:A:ARG:CA | 1:659:A:ARG:C | 6        | 1.71          |
| (1,3)   | 1:536:A:ARG:C | 1:537:A:LYS:N  | 1:537:A:LYS:CA | 1:537:A:LYS:C | 16       | 1.7           |
| (1,192) | 1:655:A:VAL:N | 1:655:A:VAL:CA | 1:655:A:VAL:C  | 1:656:A:ALA:N | 13       | 1.68          |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 4        | 1.62          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 2        | 1.57          |
| (1,160) | 1:637:A:ASN:N | 1:637:A:ASN:CA | 1:637:A:ASN:C  | 1:638:A:PHE:N | 1        | 1.55          |
| (1,21)  | 1:546:A:ALA:C | 1:547:A:ASN:N  | 1:547:A:ASN:CA | 1:547:A:ASN:C | 5        | 1.55          |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 3        | 1.54          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 17       | 1.53          |
| (1,39)  | 1:556:A:MET:C | 1:557:A:LEU:N  | 1:557:A:LEU:CA | 1:557:A:LEU:C | 11       | 1.53          |
| (1,114) | 1:607:A:PHE:N | 1:607:A:PHE:CA | 1:607:A:PHE:C  | 1:608:A:GLY:N | 8        | 1.52          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 8        | 1.52          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 19       | 1.52          |
| (1,195) | 1:659:A:ARG:C | 1:660:A:LEU:N  | 1:660:A:LEU:CA | 1:660:A:LEU:C | 4        | 1.47          |
| (1,115) | 1:612:A:LEU:C | 1:613:A:LEU:N  | 1:613:A:LEU:CA | 1:613:A:LEU:C | 7        | 1.45          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 13       | 1.44          |
| (1,74)  | 1:580:A:LYS:N | 1:580:A:LYS:CA | 1:580:A:LYS:C  | 1:581:A:MET:N | 6        | 1.4           |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 4        | 1.4           |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 6        | 1.39          |
| (1,75)  | 1:580:A:LYS:C | 1:581:A:MET:N  | 1:581:A:MET:CA | 1:581:A:MET:C | 2        | 1.37          |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 2        | 1.36          |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 15       | 1.36          |
| (1,48)  | 1:561:A:LYS:N | 1:561:A:LYS:CA | 1:561:A:LYS:C  | 1:562:A:PHE:N | 19       | 1.35          |
| (1,33)  | 1:553:A:VAL:C | 1:554:A:THR:N  | 1:554:A:THR:CA | 1:554:A:THR:C | 13       | 1.35          |
| (1,197) | 1:661:A:ASP:C | 1:662:A:ARG:N  | 1:662:A:ARG:CA | 1:662:A:ARG:C | 8        | 1.31          |
| (1,172) | 1:643:A:GLU:N | 1:643:A:GLU:CA | 1:643:A:GLU:C  | 1:644:A:GLU:N | 13       | 1.31          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 6        | 1.27          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 6        | 1.27          |
| (1,195) | 1:659:A:ARG:C | 1:660:A:LEU:N  | 1:660:A:LEU:CA | 1:660:A:LEU:C | 5        | 1.25          |
| (1,129) | 1:621:A:SER:C | 1:622:A:VAL:N  | 1:622:A:VAL:CA | 1:622:A:VAL:C | 20       | 1.25          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 10       | 1.25          |
| (1,192) | 1:655:A:VAL:N | 1:655:A:VAL:CA | 1:655:A:VAL:C  | 1:656:A:ALA:N | 10       | 1.24          |
| (1,140) | 1:627:A:TYR:N | 1:627:A:TYR:CA | 1:627:A:TYR:C  | 1:628:A:CYS:N | 1        | 1.24          |
| (1,39)  | 1:556:A:MET:C | 1:557:A:LEU:N  | 1:557:A:LEU:CA | 1:557:A:LEU:C | 16       | 1.24          |
| (1,121) | 1:617:A:ARG:C | 1:618:A:ARG:N  | 1:618:A:ARG:CA | 1:618:A:ARG:C | 8        | 1.23          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 4        | 1.23          |
| (1,144) | 1:629:A:ARG:N | 1:629:A:ARG:CA | 1:629:A:ARG:C  | 1:630:A:LEU:N | 19       | 1.22          |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 7        | 1.2           |
| (1,60)  | 1:570:A:TYR:N | 1:570:A:TYR:CA | 1:570:A:TYR:C  | 1:571:A:ILE:N | 11       | 1.2           |
| (1,106) | 1:602:A:SER:N | 1:602:A:SER:CA | 1:602:A:SER:C  | 1:603:A:ASP:N | 15       | 1.17          |
| (1,90)  | 1:591:A:VAL:N | 1:591:A:VAL:CA | 1:591:A:VAL:C  | 1:592:A:LEU:N | 5        | 1.17          |
| (1,138) | 1:626:A:THR:N | 1:626:A:THR:CA | 1:626:A:THR:C  | 1:627:A:TYR:N | 5        | 1.14          |
| (1,122) | 1:618:A:ARG:N | 1:618:A:ARG:CA | 1:618:A:ARG:C  | 1:619:A:THR:N | 3        | 1.14          |
| (1,165) | 1:639:A:ASN:C | 1:640:A:GLU:N  | 1:640:A:GLU:CA | 1:640:A:GLU:C | 5        | 1.13          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 10       | 1.12          |
| (1,95)  | 1:596:A:ASN:C | 1:597:A:LYS:N  | 1:597:A:LYS:CA | 1:597:A:LYS:C | 18       | 1.12          |
| (1,198) | 1:662:A:ARG:N | 1:662:A:ARG:CA | 1:662:A:ARG:C  | 1:663:A:ILE:N | 14       | 1.09          |

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*Continued from previous page...*

| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,128) | 1:621:A:SER:N | 1:621:A:SER:CA | 1:621:A:SER:C  | 1:622:A:VAL:N | 19       | 1.08          |
| (1,184) | 1:651:A:ALA:N | 1:651:A:ALA:CA | 1:651:A:ALA:C  | 1:652:A:PHE:N | 4        | 1.07          |
| (1,36)  | 1:555:A:ALA:N | 1:555:A:ALA:CA | 1:555:A:ALA:C  | 1:556:A:MET:N | 17       | 1.07          |
| (1,27)  | 1:550:A:PRO:C | 1:551:A:ASN:N  | 1:551:A:ASN:CA | 1:551:A:ASN:C | 10       | 1.06          |
| (1,185) | 1:651:A:ALA:C | 1:652:A:PHE:N  | 1:652:A:PHE:CA | 1:652:A:PHE:C | 18       | 1.05          |
| (1,147) | 1:630:A:LEU:C | 1:631:A:TYR:N  | 1:631:A:TYR:CA | 1:631:A:TYR:C | 20       | 1.05          |
| (1,21)  | 1:546:A:ALA:C | 1:547:A:ASN:N  | 1:547:A:ASN:CA | 1:547:A:ASN:C | 11       | 1.03          |
| (1,89)  | 1:590:A:SER:C | 1:591:A:VAL:N  | 1:591:A:VAL:CA | 1:591:A:VAL:C | 8        | 1.0           |