



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 PM UTC

PDB ID : 6NHY / pdb\_00006nhy  
BMRB ID : 30554  
Title : Structure of the transmembrane domain of the Death Receptor 5 mutant (G217Y) - Trimer Only  
Authors : Chou, J.J.; Pan, L.; Zhao, L.; Chen, W.; Piai, A.; Fu, T.; Wu, H.; Liu, Z.  
Deposited on : 2018-12-24

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

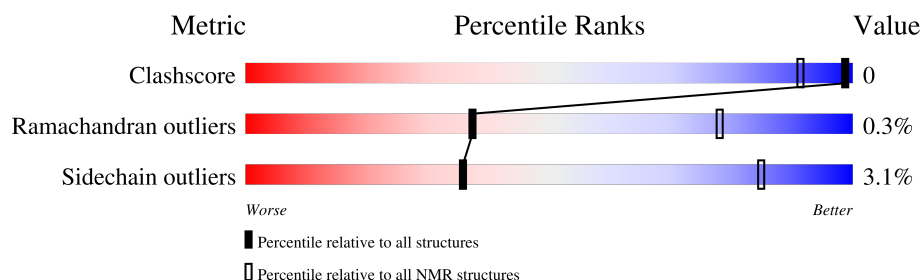
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 10%.

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     | 36     |                  |
| 1   | B     | 36     |                  |
| 1   | C     | 36     |                  |

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:212-A:236, B:212-B:236,<br>C:211-C:233 (73) | 1.00              | 1            |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1740 atoms, of which 933 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor necrosis factor receptor superfamily member 10B.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 36       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 580   | 185 | 311 | 40 | 42 | 2 |       |
| 1   | B     | 36       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 580   | 185 | 311 | 40 | 42 | 2 |       |
| 1   | C     | 36       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 580   | 185 | 311 | 40 | 42 | 2 |       |

There are 9 discrepancies between the modelled and reference sequences:

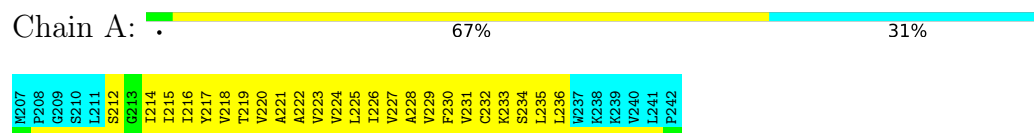
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 207     | MET      | -      | initiating methionine | UNP O14763 |
| A     | 209     | GLY      | CYS    | conflict              | UNP O14763 |
| A     | 217     | TYR      | GLY    | engineered mutation   | UNP O14763 |
| B     | 207     | MET      | -      | initiating methionine | UNP O14763 |
| B     | 209     | GLY      | CYS    | conflict              | UNP O14763 |
| B     | 217     | TYR      | GLY    | engineered mutation   | UNP O14763 |
| C     | 207     | MET      | -      | initiating methionine | UNP O14763 |
| C     | 209     | GLY      | CYS    | conflict              | UNP O14763 |
| C     | 217     | TYR      | GLY    | engineered mutation   | UNP O14763 |

## 4 Residue-property plots

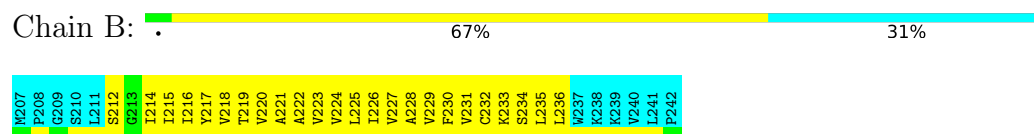
### 4.1 Average score per residue in the NMR ensemble

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

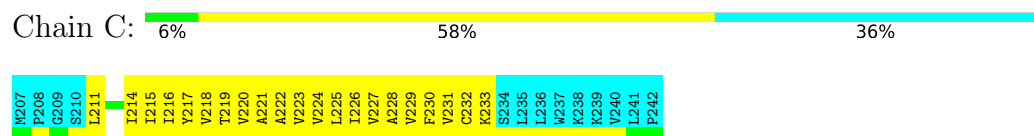
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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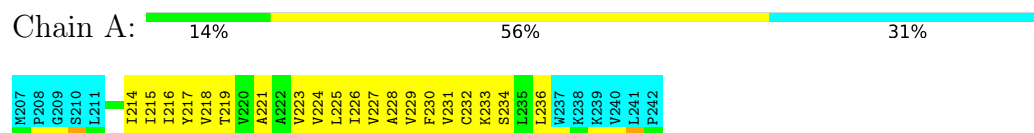


### 4.2 Scores per residue for each member of the ensemble

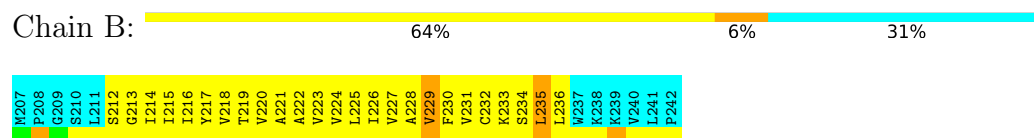
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

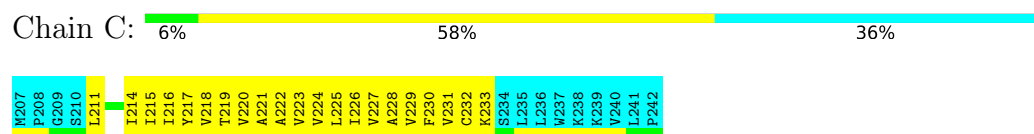
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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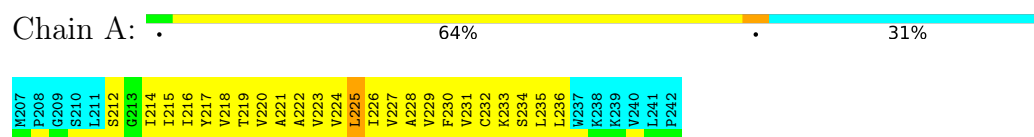


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

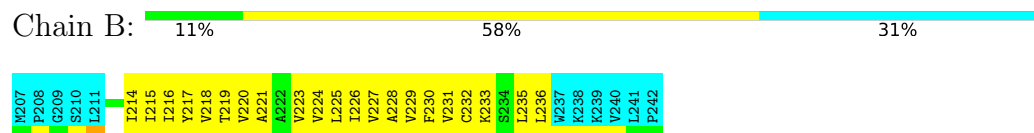


#### 4.2.2 Score per residue for model 2

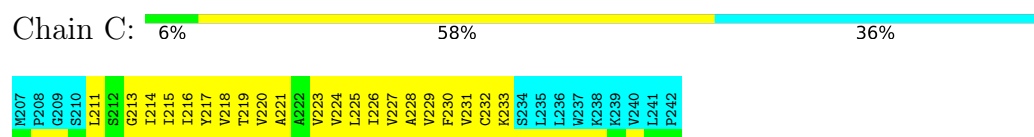
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

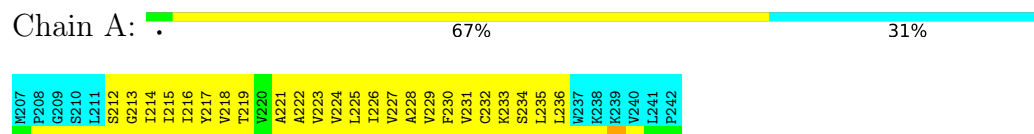


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

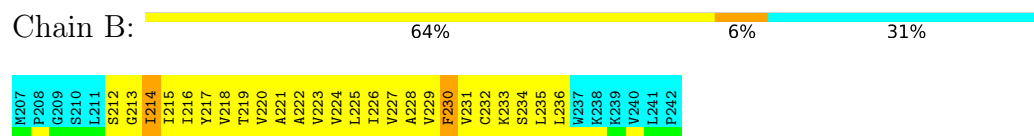


#### 4.2.3 Score per residue for model 3

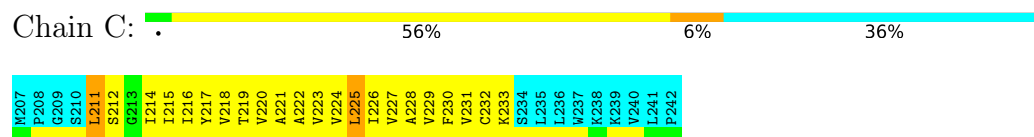
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

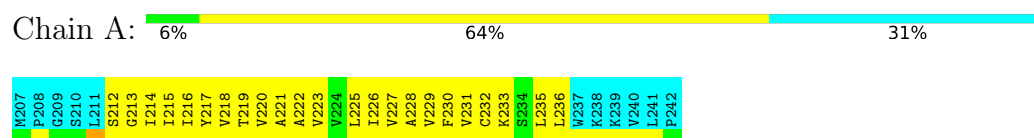


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

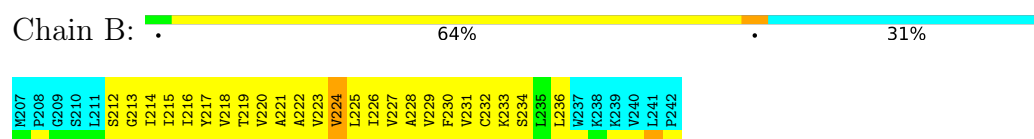


#### 4.2.4 Score per residue for model 4

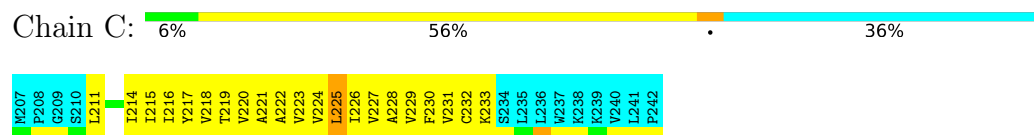
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

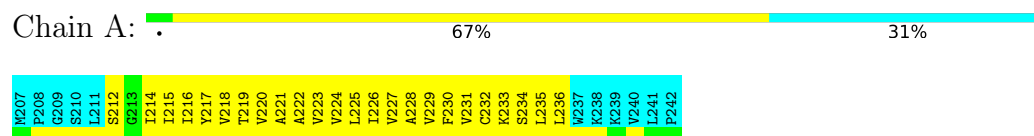


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



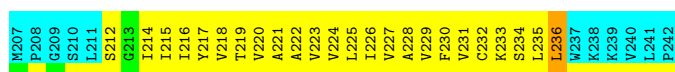
#### 4.2.5 Score per residue for model 5

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B





- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain C: 6% 58% 36%



#### 4.2.6 Score per residue for model 6

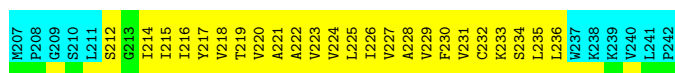
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain A: 8% 58% 31%



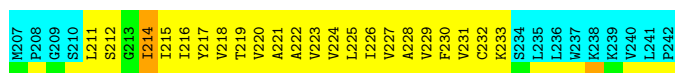
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain B: 67% 31%



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain C: 58% 36%



#### 4.2.7 Score per residue for model 7

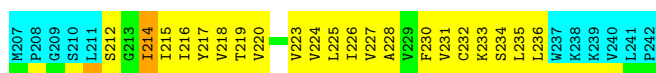
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain A: 64% 31%

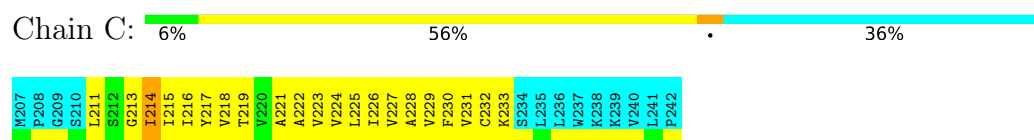


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

Chain B: 11% 56% 31%

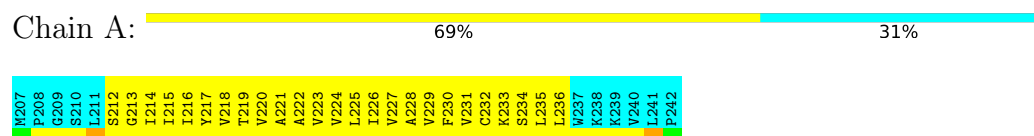


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

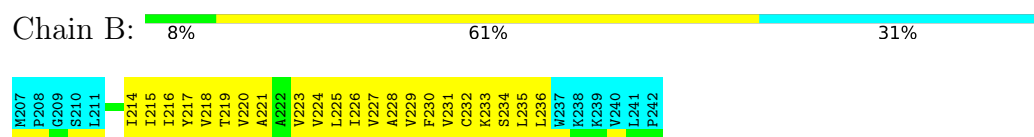


#### 4.2.8 Score per residue for model 8

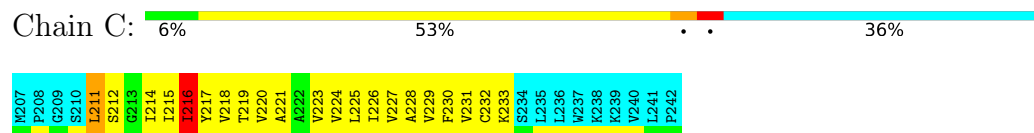
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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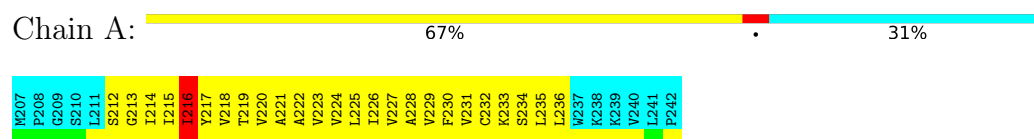


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

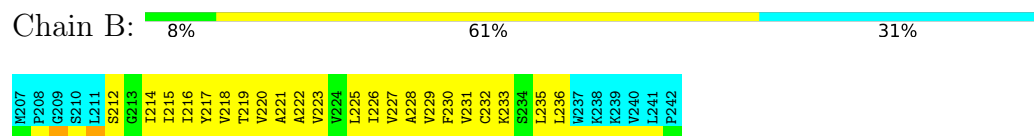


#### 4.2.9 Score per residue for model 9

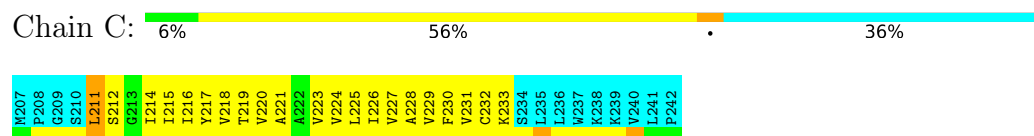
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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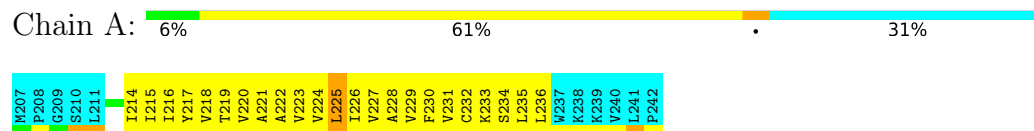


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

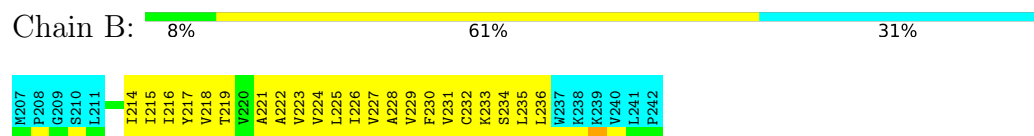


#### 4.2.10 Score per residue for model 10

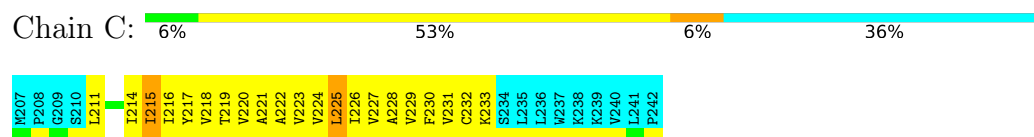
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

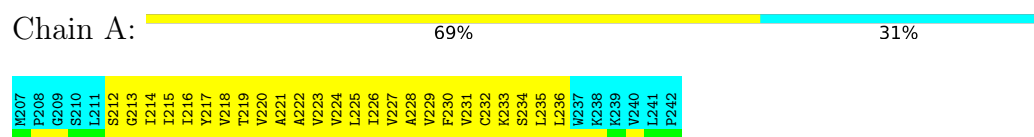


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

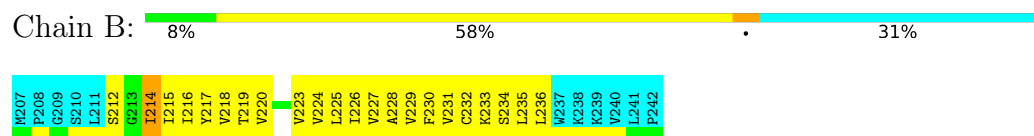


#### 4.2.11 Score per residue for model 11

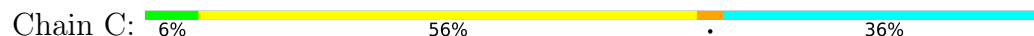
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



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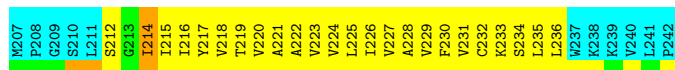
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



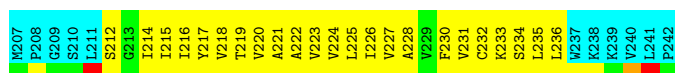
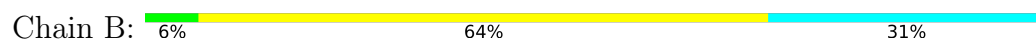


#### 4.2.12 Score per residue for model 12

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

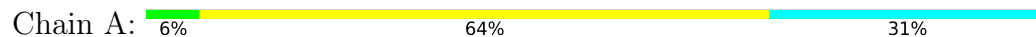


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

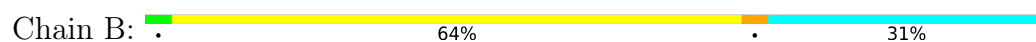


#### 4.2.13 Score per residue for model 13

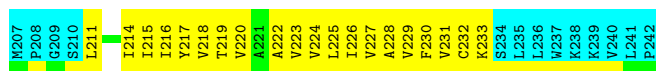
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

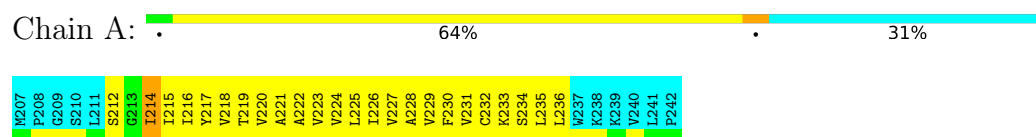


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

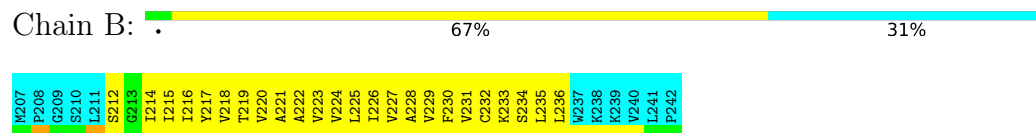


#### 4.2.14 Score per residue for model 14

- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

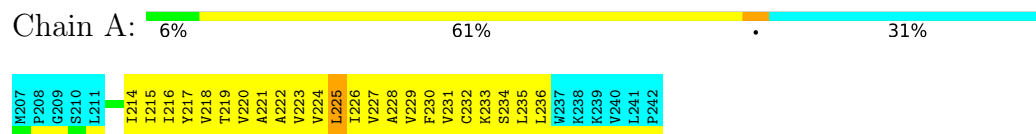


- Molecule 1: Tumor necrosis factor receptor superfamily member 10B

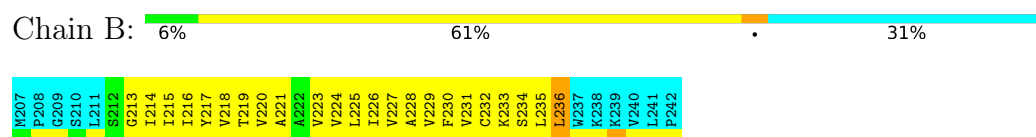


#### 4.2.15 Score per residue for model 15

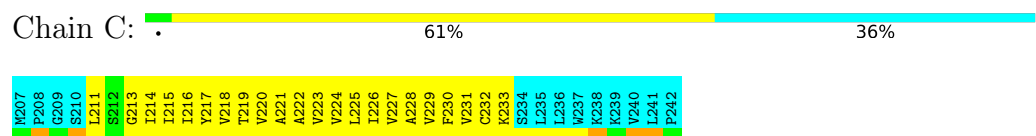
- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



- Molecule 1: Tumor necrosis factor receptor superfamily member 10B



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

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

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

| Chemical shift file(s)                       | working_cs.cif |
|----------------------------------------------|----------------|
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 133            |
| Number of shifts mapped to atoms             | 133            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 100%           |

## 6 Model quality

### 6.1 Standard geometry

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     | 3.31±0.02    | 32±2/183 ( 17.3± 1.0%) | 1.13±0.05   | 0±0/252 ( 0.0± 0.0%) |
| 1   | B     | 3.31±0.03    | 31±2/183 ( 17.2± 1.1%) | 1.11±0.04   | 0±0/252 ( 0.0± 0.0%) |
| 1   | C     | 3.32±0.02    | 30±1/169 ( 17.8± 0.8%) | 1.16±0.03   | 0±0/233 ( 0.0± 0.0%) |
| All | All   | 3.31         | 1399/8025 ( 17.4%)     | 1.14        | 0/11055 ( 0.0%)      |

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

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 214 | ILE  | CA-CB | 8.23 | 1.64        | 1.54     | 12     | 14    |
| 1   | B     | 214 | ILE  | CA-CB | 7.93 | 1.63        | 1.54     | 11     | 14    |
| 1   | B     | 218 | VAL  | N-CA  | 7.56 | 1.55        | 1.46     | 14     | 15    |
| 1   | A     | 218 | VAL  | N-CA  | 7.51 | 1.55        | 1.46     | 9      | 15    |
| 1   | A     | 227 | VAL  | N-CA  | 7.45 | 1.55        | 1.46     | 4      | 15    |
| 1   | B     | 224 | VAL  | CA-CB | 7.39 | 1.65        | 1.54     | 4      | 7     |
| 1   | C     | 230 | PHE  | N-CA  | 7.22 | 1.55        | 1.46     | 15     | 15    |
| 1   | B     | 214 | ILE  | N-CA  | 7.17 | 1.55        | 1.46     | 3      | 15    |
| 1   | C     | 214 | ILE  | N-CA  | 7.10 | 1.54        | 1.46     | 8      | 15    |
| 1   | B     | 227 | VAL  | N-CA  | 7.08 | 1.54        | 1.46     | 6      | 14    |
| 1   | A     | 230 | PHE  | N-CA  | 7.08 | 1.55        | 1.46     | 6      | 15    |
| 1   | C     | 218 | VAL  | N-CA  | 7.07 | 1.54        | 1.46     | 5      | 15    |
| 1   | A     | 235 | LEU  | N-CA  | 7.03 | 1.55        | 1.46     | 6      | 14    |
| 1   | C     | 214 | ILE  | CA-CB | 7.02 | 1.63        | 1.54     | 14     | 14    |
| 1   | C     | 215 | ILE  | N-CA  | 6.95 | 1.54        | 1.46     | 10     | 15    |
| 1   | C     | 226 | ILE  | CA-CB | 6.92 | 1.62        | 1.54     | 3      | 14    |
| 1   | C     | 227 | VAL  | N-CA  | 6.91 | 1.54        | 1.46     | 6      | 15    |
| 1   | A     | 226 | ILE  | CA-CB | 6.86 | 1.61        | 1.54     | 10     | 15    |
| 1   | A     | 229 | VAL  | N-CA  | 6.81 | 1.54        | 1.46     | 4      | 15    |
| 1   | B     | 229 | VAL  | N-CA  | 6.81 | 1.54        | 1.46     | 11     | 13    |
| 1   | A     | 214 | ILE  | N-CA  | 6.80 | 1.54        | 1.46     | 5      | 15    |
| 1   | B     | 216 | ILE  | N-CA  | 6.80 | 1.54        | 1.46     | 15     | 15    |
| 1   | B     | 228 | ALA  | N-CA  | 6.76 | 1.54        | 1.46     | 3      | 15    |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | B     | 215 | ILE  | N-CA  | 6.72 | 1.54        | 1.46     | 4      | 15    |
| 1   | A     | 236 | LEU  | N-CA  | 6.70 | 1.54        | 1.46     | 13     | 15    |
| 1   | C     | 229 | VAL  | N-CA  | 6.69 | 1.54        | 1.46     | 13     | 15    |
| 1   | A     | 215 | ILE  | N-CA  | 6.69 | 1.54        | 1.46     | 1      | 15    |
| 1   | B     | 226 | ILE  | CA-CB | 6.67 | 1.61        | 1.54     | 4      | 15    |
| 1   | C     | 225 | LEU  | N-CA  | 6.67 | 1.54        | 1.46     | 11     | 15    |
| 1   | C     | 228 | ALA  | N-CA  | 6.66 | 1.54        | 1.46     | 4      | 15    |
| 1   | C     | 216 | ILE  | N-CA  | 6.66 | 1.54        | 1.46     | 8      | 15    |
| 1   | B     | 229 | VAL  | CA-CB | 6.59 | 1.62        | 1.54     | 1      | 9     |
| 1   | A     | 226 | ILE  | N-CA  | 6.58 | 1.54        | 1.46     | 7      | 15    |
| 1   | B     | 225 | LEU  | N-CA  | 6.58 | 1.54        | 1.46     | 12     | 15    |
| 1   | B     | 236 | LEU  | N-CA  | 6.56 | 1.54        | 1.46     | 14     | 15    |
| 1   | B     | 216 | ILE  | CA-CB | 6.55 | 1.62        | 1.54     | 14     | 15    |
| 1   | A     | 216 | ILE  | N-CA  | 6.52 | 1.54        | 1.46     | 9      | 15    |
| 1   | B     | 230 | PHE  | N-CA  | 6.50 | 1.54        | 1.46     | 15     | 15    |
| 1   | C     | 231 | VAL  | N-CA  | 6.48 | 1.54        | 1.46     | 9      | 15    |
| 1   | A     | 225 | LEU  | N-CA  | 6.43 | 1.54        | 1.46     | 5      | 15    |
| 1   | A     | 228 | ALA  | N-CA  | 6.42 | 1.54        | 1.46     | 1      | 15    |
| 1   | A     | 233 | LYS  | N-CA  | 6.39 | 1.54        | 1.46     | 6      | 15    |
| 1   | C     | 215 | ILE  | CA-CB | 6.37 | 1.62        | 1.54     | 10     | 6     |
| 1   | B     | 226 | ILE  | N-CA  | 6.36 | 1.54        | 1.46     | 8      | 15    |
| 1   | B     | 235 | LEU  | N-CA  | 6.36 | 1.54        | 1.46     | 1      | 14    |
| 1   | B     | 231 | VAL  | N-CA  | 6.36 | 1.54        | 1.46     | 12     | 15    |
| 1   | B     | 219 | THR  | N-CA  | 6.34 | 1.53        | 1.46     | 1      | 15    |
| 1   | A     | 216 | ILE  | CA-CB | 6.27 | 1.61        | 1.54     | 7      | 15    |
| 1   | C     | 226 | ILE  | N-CA  | 6.26 | 1.53        | 1.46     | 6      | 15    |
| 1   | A     | 219 | THR  | N-CA  | 6.25 | 1.53        | 1.46     | 13     | 15    |
| 1   | C     | 218 | VAL  | CA-CB | 6.24 | 1.61        | 1.54     | 13     | 8     |
| 1   | A     | 224 | VAL  | N-CA  | 6.24 | 1.54        | 1.46     | 5      | 14    |
| 1   | B     | 233 | LYS  | N-CA  | 6.15 | 1.53        | 1.46     | 8      | 15    |
| 1   | C     | 217 | TYR  | N-CA  | 6.13 | 1.53        | 1.46     | 12     | 15    |
| 1   | A     | 215 | ILE  | CA-CB | 6.07 | 1.62        | 1.54     | 10     | 6     |
| 1   | C     | 233 | LYS  | N-CA  | 6.07 | 1.54        | 1.46     | 2      | 15    |
| 1   | B     | 223 | VAL  | N-CA  | 6.06 | 1.53        | 1.46     | 11     | 15    |
| 1   | C     | 219 | THR  | N-CA  | 6.04 | 1.53        | 1.46     | 1      | 15    |
| 1   | A     | 231 | VAL  | N-CA  | 6.03 | 1.53        | 1.46     | 10     | 15    |
| 1   | A     | 212 | SER  | N-CA  | 6.00 | 1.53        | 1.46     | 9      | 10    |
| 1   | C     | 223 | VAL  | N-CA  | 5.99 | 1.53        | 1.46     | 8      | 15    |
| 1   | B     | 224 | VAL  | N-CA  | 5.99 | 1.54        | 1.46     | 13     | 14    |
| 1   | B     | 232 | CYS  | N-CA  | 5.99 | 1.53        | 1.46     | 15     | 15    |
| 1   | C     | 232 | CYS  | N-CA  | 5.98 | 1.53        | 1.46     | 9      | 15    |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
|     |       |     |      |       |      |             |          | Worst  | Total |
| 1   | A     | 221 | ALA  | N-CA  | 5.98 | 1.53        | 1.46     | 13     | 15    |
| 1   | B     | 217 | TYR  | N-CA  | 5.96 | 1.53        | 1.46     | 11     | 15    |
| 1   | A     | 229 | VAL  | CA-CB | 5.96 | 1.62        | 1.54     | 12     | 7     |
| 1   | A     | 232 | CYS  | N-CA  | 5.95 | 1.53        | 1.46     | 5      | 15    |
| 1   | C     | 211 | LEU  | N-CA  | 5.93 | 1.53        | 1.46     | 14     | 14    |
| 1   | C     | 216 | ILE  | CA-CB | 5.93 | 1.62        | 1.54     | 9      | 15    |
| 1   | A     | 218 | VAL  | CA-CB | 5.91 | 1.61        | 1.54     | 15     | 9     |
| 1   | A     | 223 | VAL  | N-CA  | 5.91 | 1.53        | 1.46     | 11     | 15    |
| 1   | B     | 234 | SER  | N-CA  | 5.90 | 1.53        | 1.46     | 3      | 12    |
| 1   | A     | 223 | VAL  | CA-CB | 5.88 | 1.61        | 1.54     | 6      | 15    |
| 1   | B     | 218 | VAL  | CA-CB | 5.87 | 1.61        | 1.54     | 10     | 6     |
| 1   | C     | 224 | VAL  | N-CA  | 5.86 | 1.53        | 1.46     | 9      | 14    |
| 1   | A     | 217 | TYR  | N-CA  | 5.83 | 1.53        | 1.46     | 3      | 15    |
| 1   | C     | 220 | VAL  | N-CA  | 5.83 | 1.53        | 1.46     | 9      | 11    |
| 1   | A     | 227 | VAL  | CA-CB | 5.82 | 1.61        | 1.54     | 3      | 15    |
| 1   | C     | 220 | VAL  | CA-CB | 5.82 | 1.61        | 1.54     | 10     | 10    |
| 1   | C     | 231 | VAL  | CA-CB | 5.80 | 1.61        | 1.54     | 9      | 9     |
| 1   | C     | 211 | LEU  | CB-CG | 5.80 | 1.65        | 1.53     | 2      | 7     |
| 1   | A     | 234 | SER  | N-CA  | 5.79 | 1.53        | 1.46     | 1      | 14    |
| 1   | B     | 220 | VAL  | N-CA  | 5.79 | 1.53        | 1.46     | 13     | 12    |
| 1   | B     | 215 | ILE  | CA-CB | 5.78 | 1.62        | 1.54     | 9      | 6     |
| 1   | C     | 229 | VAL  | CA-CB | 5.78 | 1.61        | 1.54     | 7      | 9     |
| 1   | B     | 220 | VAL  | CA-CB | 5.76 | 1.61        | 1.54     | 9      | 7     |
| 1   | B     | 230 | PHE  | CA-CB | 5.75 | 1.62        | 1.53     | 3      | 1     |
| 1   | C     | 227 | VAL  | CA-CB | 5.72 | 1.61        | 1.54     | 6      | 15    |
| 1   | C     | 211 | LEU  | CA-CB | 5.69 | 1.61        | 1.53     | 15     | 3     |
| 1   | B     | 212 | SER  | N-CA  | 5.64 | 1.53        | 1.46     | 9      | 11    |
| 1   | B     | 223 | VAL  | CA-CB | 5.64 | 1.61        | 1.54     | 7      | 15    |
| 1   | A     | 220 | VAL  | N-CA  | 5.63 | 1.53        | 1.46     | 4      | 11    |
| 1   | B     | 222 | ALA  | N-CA  | 5.62 | 1.53        | 1.46     | 4      | 10    |
| 1   | A     | 220 | VAL  | CA-CB | 5.61 | 1.61        | 1.54     | 11     | 3     |
| 1   | B     | 227 | VAL  | CA-CB | 5.61 | 1.61        | 1.54     | 6      | 15    |
| 1   | C     | 223 | VAL  | CA-CB | 5.61 | 1.61        | 1.54     | 9      | 15    |
| 1   | A     | 222 | ALA  | N-CA  | 5.60 | 1.53        | 1.46     | 3      | 12    |
| 1   | C     | 212 | SER  | N-CA  | 5.58 | 1.53        | 1.46     | 5      | 6     |
| 1   | B     | 231 | VAL  | CA-CB | 5.58 | 1.61        | 1.54     | 12     | 11    |
| 1   | A     | 235 | LEU  | CB-CG | 5.57 | 1.64        | 1.53     | 8      | 1     |
| 1   | A     | 231 | VAL  | CA-CB | 5.54 | 1.61        | 1.54     | 14     | 7     |
| 1   | C     | 225 | LEU  | CB-CG | 5.52 | 1.64        | 1.53     | 4      | 4     |
| 1   | C     | 221 | ALA  | N-CA  | 5.52 | 1.53        | 1.46     | 15     | 14    |
| 1   | C     | 222 | ALA  | N-CA  | 5.41 | 1.52        | 1.46     | 3      | 11    |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
|     |       |     |      |        |      |             |          | Worst  | Total |
| 1   | C     | 233 | LYS  | CA-CB  | 5.39 | 1.62        | 1.53     | 2      | 1     |
| 1   | B     | 236 | LEU  | CA-CB  | 5.39 | 1.62        | 1.53     | 15     | 2     |
| 1   | B     | 235 | LEU  | CB-CG  | 5.38 | 1.64        | 1.53     | 14     | 1     |
| 1   | A     | 225 | LEU  | CA-CB  | 5.35 | 1.61        | 1.53     | 15     | 3     |
| 1   | C     | 225 | LEU  | CA-CB  | 5.33 | 1.61        | 1.53     | 10     | 4     |
| 1   | B     | 235 | LEU  | CA-CB  | 5.33 | 1.62        | 1.53     | 8      | 2     |
| 1   | B     | 221 | ALA  | N-CA   | 5.32 | 1.52        | 1.46     | 6      | 13    |
| 1   | B     | 213 | GLY  | N-CA   | 5.32 | 1.52        | 1.45     | 13     | 5     |
| 1   | C     | 224 | VAL  | CA-CB  | 5.28 | 1.61        | 1.54     | 1      | 5     |
| 1   | A     | 236 | LEU  | CA-CB  | 5.23 | 1.61        | 1.53     | 6      | 1     |
| 1   | A     | 213 | GLY  | N-CA   | 5.23 | 1.52        | 1.45     | 11     | 6     |
| 1   | A     | 230 | PHE  | CA-CB  | 5.21 | 1.61        | 1.53     | 1      | 1     |
| 1   | A     | 224 | VAL  | CA-CB  | 5.21 | 1.61        | 1.54     | 12     | 5     |
| 1   | A     | 235 | LEU  | CA-CB  | 5.17 | 1.61        | 1.53     | 11     | 1     |
| 1   | A     | 225 | LEU  | CB-CG  | 5.11 | 1.63        | 1.53     | 15     | 3     |
| 1   | B     | 225 | LEU  | CA-CB  | 5.11 | 1.61        | 1.53     | 13     | 1     |
| 1   | A     | 214 | ILE  | CB-CG1 | 5.06 | 1.63        | 1.53     | 14     | 2     |
| 1   | C     | 213 | GLY  | N-CA   | 5.05 | 1.52        | 1.45     | 7      | 3     |
| 1   | B     | 225 | LEU  | CB-CG  | 5.04 | 1.63        | 1.53     | 13     | 1     |
| 1   | B     | 214 | ILE  | CB-CG1 | 5.02 | 1.63        | 1.53     | 12     | 1     |
| 1   | A     | 233 | LYS  | CA-CB  | 5.01 | 1.61        | 1.53     | 15     | 1     |

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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   | B     | 181   | 211      | 211      | 0±0     |
| 1   | C     | 167   | 195      | 195      | 0±0     |
| 1   | A     | 181   | 211      | 211      | 0±0     |
| All | All   | 7935  | 9255     | 9255     | 2       |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 0.

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

| Atom-1           | Atom-2        | Clash(Å) | Distance(Å) | Models |       |
|------------------|---------------|----------|-------------|--------|-------|
|                  |               |          |             | Worst  | Total |
| 1:C:216:ILE:HD12 | 1:C:216:ILE:N | 0.43     | 2.29        | 8      | 1     |
| 1:A:216:ILE:HD12 | 1:A:216:ILE:N | 0.42     | 2.29        | 9      | 1     |

## 6.3 Torsion angles [i](#)

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

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

| Mol | Chain | Analysed        | Favoured      | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|---------------|------------|------------|-------------|-----|
| 1   | A     | 25/36 (69%)     | 25±0 (100±0%) | 0±0 (0±0%) | 0±0 (0±0%) | 100         | 100 |
| 1   | B     | 25/36 (69%)     | 25±0 (100±0%) | 0±0 (0±0%) | 0±0 (0±0%) | 100         | 100 |
| 1   | C     | 23/36 (64%)     | 22±0 (98±2%)  | 0±0 (1±2%) | 0±0 (1±2%) | 16          | 66  |
| All | All   | 1095/1620 (68%) | 1087 (99%)    | 5 (0%)     | 3 (0%)     | 37          | 78  |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | C     | 211 | LEU  | 3              |

### 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     | 21/31 (68%)    | 20±0 (97±2%) | 1±0 (3±2%) | 42          | 88 |
| 1   | B     | 21/31 (68%)    | 20±1 (97±3%) | 1±1 (3±3%) | 35          | 84 |
| 1   | C     | 19/31 (61%)    | 18±1 (96±4%) | 1±1 (4±4%) | 32          | 82 |
| All | All   | 915/1395 (66%) | 887 (97%)    | 28 (3%)    | 36          | 85 |

All 17 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   | C     | 225 | LEU  | 4              |
| 1   | A     | 225 | LEU  | 3              |
| 1   | B     | 214 | ILE  | 3              |
| 1   | C     | 214 | ILE  | 3              |
| 1   | B     | 236 | LEU  | 2              |
| 1   | A     | 214 | ILE  | 2              |
| 1   | B     | 229 | VAL  | 1              |
| 1   | B     | 235 | LEU  | 1              |
| 1   | B     | 230 | PHE  | 1              |
| 1   | B     | 224 | VAL  | 1              |
| 1   | A     | 233 | LYS  | 1              |
| 1   | A     | 235 | LEU  | 1              |
| 1   | C     | 211 | LEU  | 1              |
| 1   | C     | 216 | ILE  | 1              |
| 1   | A     | 216 | ILE  | 1              |
| 1   | C     | 215 | ILE  | 1              |
| 1   | B     | 225 | LEU  | 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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 10% for the well-defined parts and 9% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `bmr.b.txt`

#### 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                  | 133 |
| Number of shifts mapped to atoms        | 133 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 34       | $-0.06 \pm 0.18$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 0        | —                               | None (insufficient data)   |
| $^{13}\text{C}'$       | 33       | $0.43 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 33       | $1.01 \pm 0.47$                 | Should be applied          |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 100 atoms were assigned a chemical shift out of a possible 1030. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$ | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|--------------|-----------------|-----------------|
| Backbone  | 100/368 (27%) | 25/149 (17%) | 50/146 (34%)    | 25/73 (34%)     |
| Sidechain | 0/605 (0%)    | 0/418 (0%)   | 0/184 (0%)      | 0/3 (0%)        |

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|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 0/57 (0%)      | 0/27 (0%)      | 0/30 (0%)       | 0/0 (—%)        |
| Overall  | 100/1030 (10%) | 25/594 (4%)    | 50/360 (14%)    | 25/76 (33%)     |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 133 atoms were assigned a chemical shift out of a possible 1536. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 133/534 (25%) | 33/216 (15%)   | 67/216 (31%)    | 33/102 (32%)    |
| Sidechain | 0/909 (0%)    | 0/621 (0%)     | 0/279 (0%)      | 0/9 (0%)        |
| Aromatic  | 0/93 (0%)     | 0/45 (0%)      | 0/45 (0%)       | 0/3 (0%)        |
| Overall   | 133/1536 (9%) | 33/882 (4%)    | 67/540 (12%)    | 33/114 (29%)    |

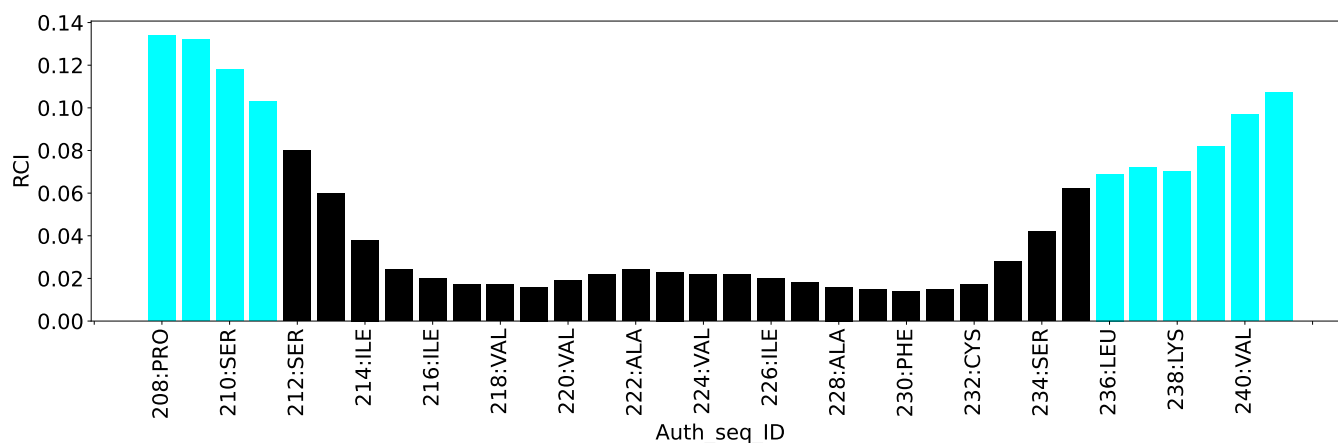
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 378   |
| Intra-residue ( $ i-j =0$ )                              | 84    |
| Sequential ( $ i-j =1$ )                                 | 165   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 126   |
| Long range ( $ i-j \geq 5$ )                             | 3     |
| Inter-chain                                              | 0     |
| Hydrogen bond restraints                                 | 0     |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 56    |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 4.0   |
| Number of long range restraints per residue <sup>1</sup> | 0.0   |

<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)  | 34.2                                   | 0.2     |
| 0.2-0.5 (Medium) | 44.2                                   | 0.5     |
| >0.5 (Large)     | 12.4                                   | 5.17    |

### 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)   | 4.7                                    | 2.67    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

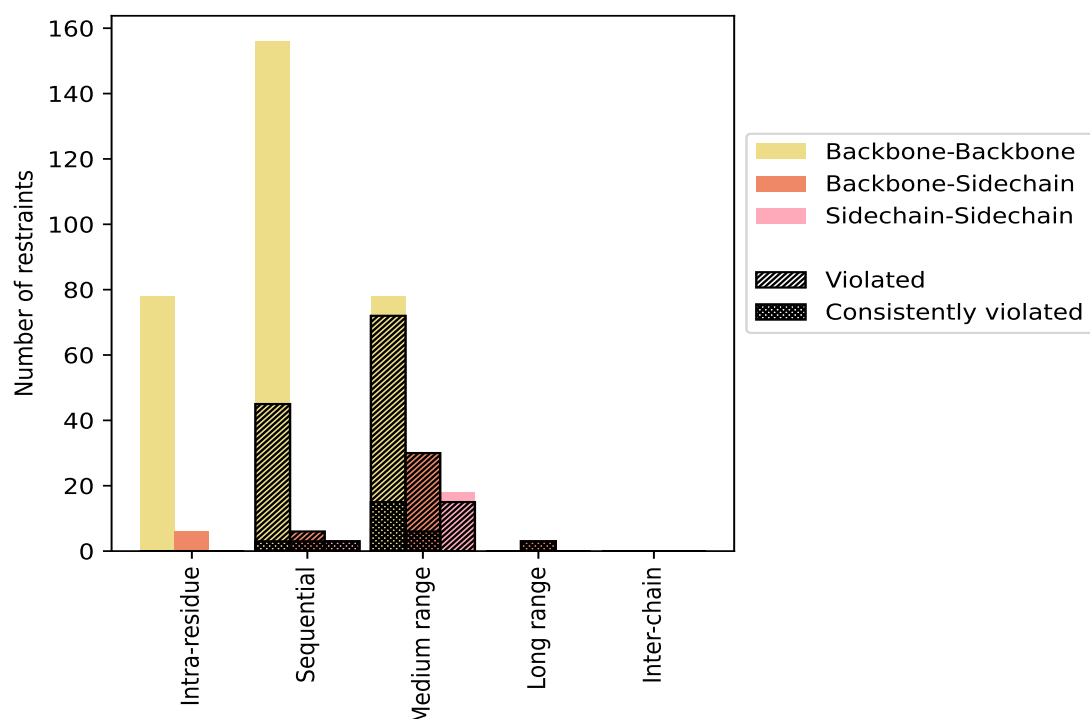
### 9.1 Summary of distance violations ⓘ

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>84</b>  | <b>22.2</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                                                           | 78         | 20.6           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 6          | 1.6            | 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>Sequential (<math> i-j =1</math>)</b>                                    | <b>165</b> | <b>43.7</b>    | <b>54</b>             | <b>32.7</b>    | <b>14.3</b>    | <b>9</b>                           | <b>5.5</b>     | <b>2.4</b>     |
| Backbone-Backbone                                                           | 156        | 41.3           | 45                    | 28.8           | 11.9           | 3                                  | 1.9            | 0.8            |
| Backbone-Sidechain                                                          | 6          | 1.6            | 6                     | 100.0          | 1.6            | 3                                  | 50.0           | 0.8            |
| Sidechain-Sidechain                                                         | 3          | 0.8            | 3                     | 100.0          | 0.8            | 3                                  | 100.0          | 0.8            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>126</b> | <b>33.3</b>    | <b>117</b>            | <b>92.9</b>    | <b>31.0</b>    | <b>21</b>                          | <b>16.7</b>    | <b>5.6</b>     |
| Backbone-Backbone                                                           | 78         | 20.6           | 72                    | 92.3           | 19.0           | 15                                 | 19.2           | 4.0            |
| Backbone-Sidechain                                                          | 30         | 7.9            | 30                    | 100.0          | 7.9            | 6                                  | 20.0           | 1.6            |
| Sidechain-Sidechain                                                         | 18         | 4.8            | 15                    | 83.3           | 4.0            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>3</b>   | <b>0.8</b>     | <b>3</b>              | <b>100.0</b>   | <b>0.8</b>     | <b>3</b>                           | <b>100.0</b>   | <b>0.8</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 3          | 0.8            | 3                     | 100.0          | 0.8            | 3                                  | 100.0          | 0.8            |
| Sidechain-Sidechain                                                         | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 0          | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>   | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>378</b> | <b>100.0</b>   | <b>174</b>            | <b>46.0</b>    | <b>46.0</b>    | <b>33</b>                          | <b>8.7</b>     | <b>8.7</b>     |
| Backbone-Backbone                                                           | 312        | 82.5           | 117                   | 37.5           | 31.0           | 18                                 | 5.8            | 4.8            |
| Backbone-Sidechain                                                          | 45         | 11.9           | 39                    | 86.7           | 10.3           | 12                                 | 26.7           | 3.2            |
| Sidechain-Sidechain                                                         | 21         | 5.6            | 18                    | 85.7           | 4.8            | 3                                  | 14.3           | 0.8            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 0                    | 24              | 57              | 3               | 0               | 84    | 0.4      | 2.94    | 0.54                | 0.24       |
| 2        | 0                    | 27              | 57              | 3               | 0               | 87    | 0.35     | 2.96    | 0.52                | 0.19       |
| 3        | 0                    | 30              | 69              | 3               | 0               | 102   | 0.39     | 3.0     | 0.52                | 0.25       |
| 4        | 0                    | 30              | 66              | 3               | 0               | 99    | 0.37     | 2.99    | 0.52                | 0.27       |
| 5        | 0                    | 30              | 63              | 3               | 0               | 96    | 0.38     | 2.93    | 0.51                | 0.24       |
| 6        | 0                    | 24              | 63              | 3               | 0               | 90    | 0.36     | 2.91    | 0.49                | 0.29       |
| 7        | 0                    | 21              | 54              | 3               | 0               | 78    | 0.45     | 2.97    | 0.56                | 0.31       |
| 8        | 0                    | 24              | 72              | 3               | 0               | 99    | 0.6      | 5.17    | 0.93                | 0.33       |
| 9        | 0                    | 27              | 60              | 3               | 0               | 90    | 0.36     | 2.97    | 0.51                | 0.25       |
| 10       | 0                    | 18              | 57              | 3               | 0               | 78    | 0.44     | 2.94    | 0.57                | 0.26       |

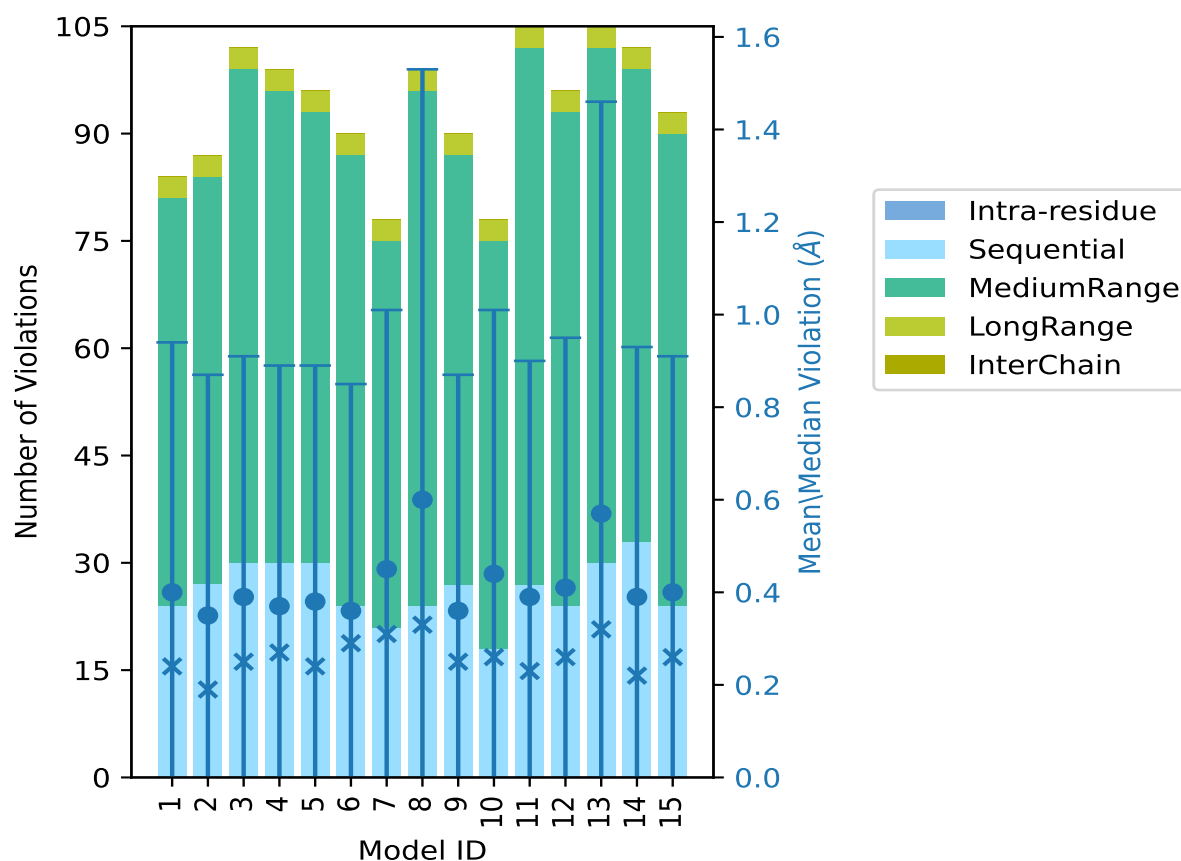
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| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 0                    | 27              | 75              | 3               | 0               | 105   | 0.39     | 2.91    | 0.51                | 0.23       |
| 12       | 0                    | 24              | 69              | 3               | 0               | 96    | 0.41     | 3.11    | 0.54                | 0.26       |
| 13       | 0                    | 30              | 72              | 3               | 0               | 105   | 0.57     | 4.97    | 0.89                | 0.32       |
| 14       | 0                    | 33              | 66              | 3               | 0               | 102   | 0.39     | 3.09    | 0.54                | 0.22       |
| 15       | 0                    | 24              | 66              | 3               | 0               | 93    | 0.4      | 2.88    | 0.51                | 0.26       |

<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

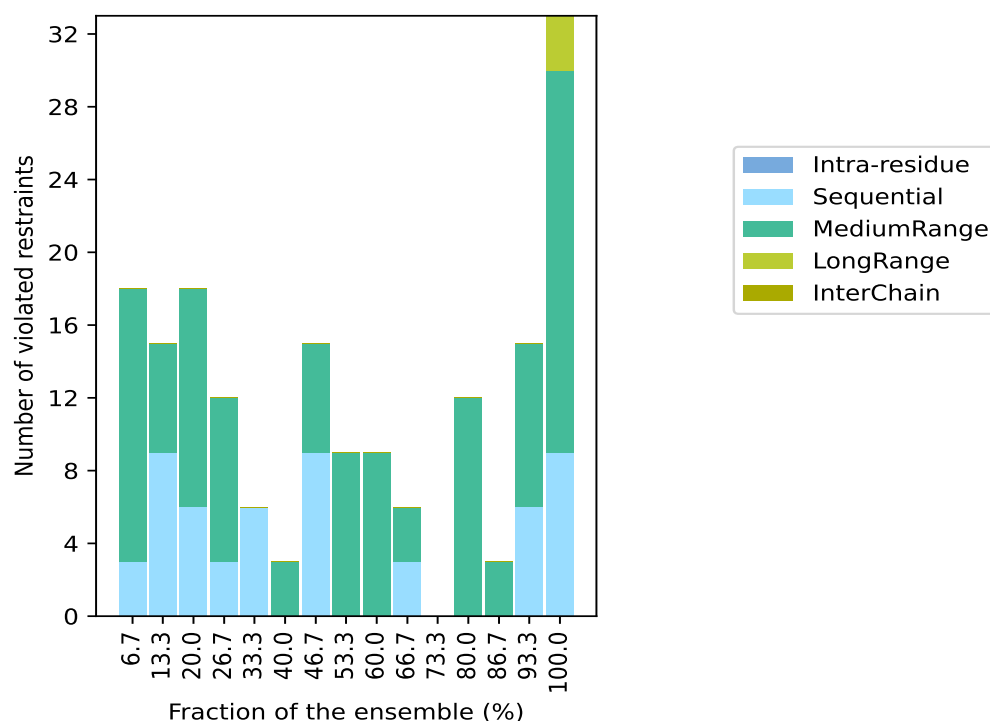
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 204(IR:84, SQ:111, MR:9, LR:0, IC:0) restraints are not violated 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>       | %     |
| 0                             | 3               | 15              | 0               | 0               | 18    | 1                        | 6.7   |
| 0                             | 9               | 6               | 0               | 0               | 15    | 2                        | 13.3  |
| 0                             | 6               | 12              | 0               | 0               | 18    | 3                        | 20.0  |
| 0                             | 3               | 9               | 0               | 0               | 12    | 4                        | 26.7  |
| 0                             | 6               | 0               | 0               | 0               | 6     | 5                        | 33.3  |
| 0                             | 0               | 3               | 0               | 0               | 3     | 6                        | 40.0  |
| 0                             | 9               | 6               | 0               | 0               | 15    | 7                        | 46.7  |
| 0                             | 0               | 9               | 0               | 0               | 9     | 8                        | 53.3  |
| 0                             | 0               | 9               | 0               | 0               | 9     | 9                        | 60.0  |
| 0                             | 3               | 3               | 0               | 0               | 6     | 10                       | 66.7  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 11                       | 73.3  |
| 0                             | 0               | 12              | 0               | 0               | 12    | 12                       | 80.0  |
| 0                             | 0               | 3               | 0               | 0               | 3     | 13                       | 86.7  |
| 0                             | 6               | 9               | 0               | 0               | 15    | 14                       | 93.3  |
| 0                             | 9               | 21              | 3               | 0               | 33    | 15                       | 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

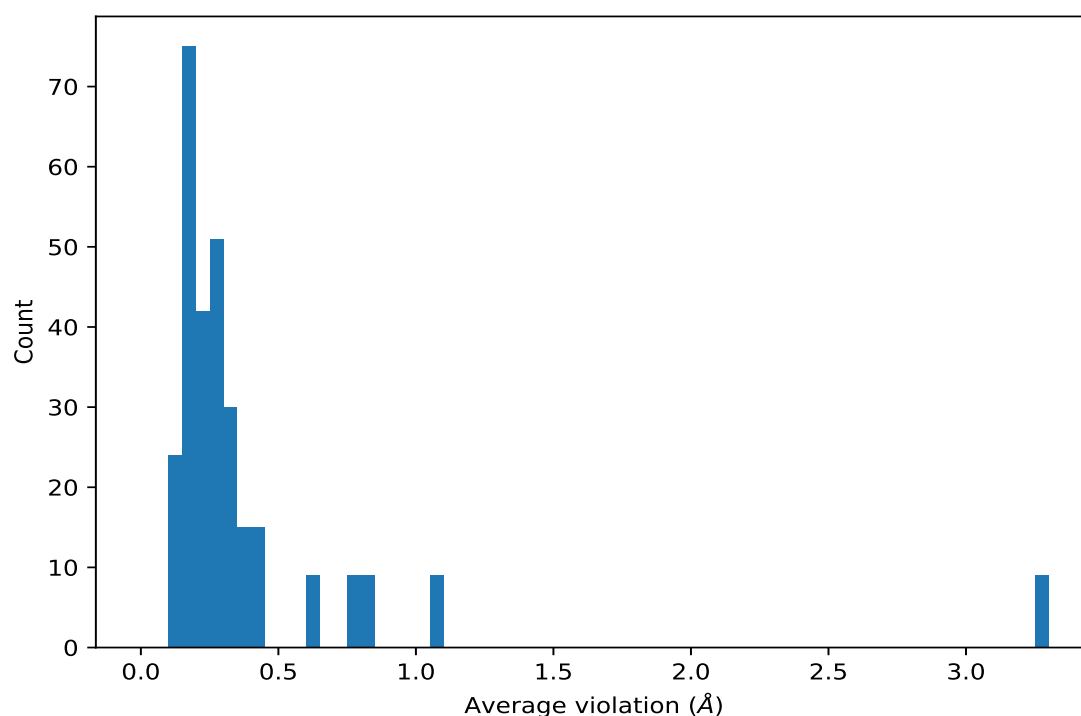
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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) |
|---------|------------------|----------------|---------------------|----------|---------------------|------------|
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 15                  | 3.25     | 0.72                | 2.97       |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG | 15                  | 1.09     | 0.28                | 1.05       |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG | 15                  | 1.09     | 0.28                | 1.05       |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG | 15                  | 1.09     | 0.28                | 1.05       |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG | 15                  | 1.09     | 0.28                | 1.05       |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG | 15                  | 1.09     | 0.28                | 1.05       |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG | 15                  | 1.09     | 0.28                | 1.05       |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG | 15                  | 1.09     | 0.28                | 1.05       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 15                  | 1.09     | 0.28                | 1.05       |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 15                  | 1.09     | 0.28                | 1.05       |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 15                  | 0.81     | 0.41                | 1.03       |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 15                  | 0.64     | 0.47                | 0.46       |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 15                  | 0.41     | 0.21                | 0.35       |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 15                  | 0.41     | 0.21                | 0.35       |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 15                  | 0.41     | 0.21                | 0.35       |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA   | 15                  | 0.41     | 0.06                | 0.43       |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA   | 15                  | 0.41     | 0.06                | 0.43       |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA   | 15                  | 0.41     | 0.06                | 0.43       |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA   | 15                  | 0.34     | 0.04                | 0.34       |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA   | 15                  | 0.34     | 0.04                | 0.34       |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA   | 15                  | 0.34     | 0.04                | 0.34       |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 15                  | 0.33     | 0.13                | 0.27       |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 15                  | 0.33     | 0.13                | 0.27       |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 15                  | 0.33     | 0.13                | 0.27       |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 15                  | 0.32     | 0.07                | 0.32       |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 15                  | 0.32     | 0.07                | 0.32       |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 15                  | 0.32     | 0.07                | 0.32       |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA   | 15                  | 0.29     | 0.08                | 0.3        |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA   | 15                  | 0.29     | 0.08                | 0.3        |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA   | 15                  | 0.29     | 0.08                | 0.3        |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA   | 15                  | 0.29     | 0.08                | 0.3        |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA   | 15                  | 0.29     | 0.08                | 0.3        |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA   | 15                  | 0.29     | 0.08                | 0.3        |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA   | 15                  | 0.29     | 0.08                | 0.3        |

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| Key     | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 15                  | 0.29     | 0.08                | 0.3        |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 15                  | 0.29     | 0.08                | 0.3        |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 15                  | 0.17     | 0.03                | 0.16       |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 15                  | 0.17     | 0.03                | 0.16       |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 15                  | 0.17     | 0.03                | 0.16       |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 14                  | 0.37     | 0.1                 | 0.36       |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 14                  | 0.37     | 0.1                 | 0.36       |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 14                  | 0.37     | 0.1                 | 0.36       |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 14                  | 0.31     | 0.11                | 0.3        |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 14                  | 0.31     | 0.11                | 0.3        |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 14                  | 0.31     | 0.11                | 0.3        |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 14                  | 0.3      | 0.13                | 0.32       |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 14                  | 0.3      | 0.13                | 0.32       |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 14                  | 0.3      | 0.13                | 0.32       |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 14                  | 0.16     | 0.01                | 0.16       |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 14                  | 0.16     | 0.01                | 0.16       |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 14                  | 0.16     | 0.01                | 0.16       |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 14                  | 0.11     | 0.01                | 0.11       |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 13                  | 0.22     | 0.08                | 0.22       |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 13                  | 0.22     | 0.08                | 0.22       |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 13                  | 0.22     | 0.08                | 0.22       |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 12                  | 0.35     | 0.17                | 0.39       |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 12                  | 0.35     | 0.17                | 0.39       |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 12                  | 0.35     | 0.17                | 0.39       |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 12                  | 0.32     | 0.14                | 0.29       |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 12                  | 0.32     | 0.14                | 0.29       |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 12                  | 0.32     | 0.14                | 0.29       |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 12                  | 0.32     | 0.14                | 0.29       |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 12                  | 0.32     | 0.14                | 0.29       |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 12                  | 0.32     | 0.14                | 0.29       |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 12                  | 0.3      | 0.12                | 0.29       |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 12                  | 0.3      | 0.12                | 0.29       |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 12                  | 0.3      | 0.12                | 0.29       |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 12                  | 0.18     | 0.09                | 0.16       |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 12                  | 0.18     | 0.09                | 0.16       |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 12                  | 0.18     | 0.09                | 0.16       |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 10                  | 0.25     | 0.08                | 0.29       |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 10                  | 0.25     | 0.08                | 0.29       |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 10                  | 0.25     | 0.08                | 0.29       |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |

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| Key     | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 10                  | 0.18     | 0.05                | 0.17       |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 9                   | 0.4      | 0.28                | 0.32       |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 9                   | 0.28     | 0.08                | 0.28       |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 9                   | 0.28     | 0.08                | 0.28       |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 9                   | 0.28     | 0.08                | 0.28       |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 9                   | 0.19     | 0.05                | 0.19       |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 9                   | 0.19     | 0.05                | 0.19       |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 9                   | 0.19     | 0.05                | 0.19       |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 8                   | 0.26     | 0.1                 | 0.28       |

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| Key     | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2  | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3  | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2  | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3  | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2  | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3  | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2  | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3  | 8                   | 0.26     | 0.1                 | 0.28       |
| (1,86)  | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,86)  | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,86)  | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 8                   | 0.2      | 0.06                | 0.22       |
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 8                   | 0.19     | 0.08                | 0.18       |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 8                   | 0.19     | 0.08                | 0.18       |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 8                   | 0.19     | 0.08                | 0.18       |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 7                   | 0.75     | 0.91                | 0.21       |
| (1,92)  | 1:231:C:VAL:H    | 1:228:C:ALA:HA   | 7                   | 0.34     | 0.15                | 0.27       |
| (1,211) | 1:231:C:VAL:H    | 1:228:C:ALA:HA   | 7                   | 0.34     | 0.15                | 0.27       |
| (1,330) | 1:231:C:VAL:H    | 1:228:C:ALA:HA   | 7                   | 0.34     | 0.15                | 0.27       |
| (1,75)  | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,75)  | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,75)  | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,194) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,194) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,194) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,313) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,313) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,313) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA   | 7                   | 0.2      | 0.08                | 0.18       |
| (1,41)  | 1:220:C:VAL:H    | 1:219:C:THR:HA   | 7                   | 0.13     | 0.0                 | 0.13       |

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| Key     | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,160) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 7                   | 0.13     | 0.0                 | 0.13       |
| (1,279) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 7                   | 0.13     | 0.0                 | 0.13       |
| (1,93)  | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,212) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,331) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 7                   | 0.12     | 0.01                | 0.12       |
| (1,76)  | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,76)  | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,76)  | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,195) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,195) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,195) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,314) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,314) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,314) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 6                   | 0.36     | 0.04                | 0.36       |
| (1,68)  | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,187) | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,306) | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 5                   | 0.12     | 0.02                | 0.11       |
| (1,18)  | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,137) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,256) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 5                   | 0.12     | 0.01                | 0.12       |
| (1,70)  | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,70)  | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,70)  | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,70)  | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,70)  | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,70)  | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 4                   | 0.19     | 0.06                | 0.18       |
| (1,77)  | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 4                   | 0.18     | 0.07                | 0.16       |
| (1,196) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 4                   | 0.18     | 0.07                | 0.16       |
| (1,315) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 4                   | 0.18     | 0.07                | 0.16       |
| (1,97)  | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |

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| Key     | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,97)  | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,97)  | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,216) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,216) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,216) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,335) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,335) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,335) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 4                   | 0.15     | 0.02                | 0.16       |
| (1,56)  | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 4                   | 0.11     | 0.01                | 0.12       |
| (1,175) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 4                   | 0.11     | 0.01                | 0.12       |
| (1,294) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 4                   | 0.11     | 0.01                | 0.12       |
| (1,117) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA  | 3                   | 0.33     | 0.09                | 0.37       |
| (1,236) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA  | 3                   | 0.33     | 0.09                | 0.37       |
| (1,355) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA  | 3                   | 0.33     | 0.09                | 0.37       |
| (1,15)  | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,15)  | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,15)  | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,15)  | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,15)  | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,15)  | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,134) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,134) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,134) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,134) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,134) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,134) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,253) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,253) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,253) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,253) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,253) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,253) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 3                   | 0.27     | 0.21                | 0.12       |
| (1,14)  | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA  | 3                   | 0.22     | 0.09                | 0.16       |
| (1,14)  | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA  | 3                   | 0.22     | 0.09                | 0.16       |
| (1,14)  | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA  | 3                   | 0.22     | 0.09                | 0.16       |
| (1,115) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 3                   | 0.22     | 0.07                | 0.23       |
| (1,133) | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA  | 3                   | 0.22     | 0.09                | 0.16       |
| (1,133) | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA  | 3                   | 0.22     | 0.09                | 0.16       |
| (1,133) | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA  | 3                   | 0.22     | 0.09                | 0.16       |
| (1,234) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 3                   | 0.22     | 0.07                | 0.23       |
| (1,252) | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA  | 3                   | 0.22     | 0.09                | 0.16       |
| (1,252) | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA  | 3                   | 0.22     | 0.09                | 0.16       |

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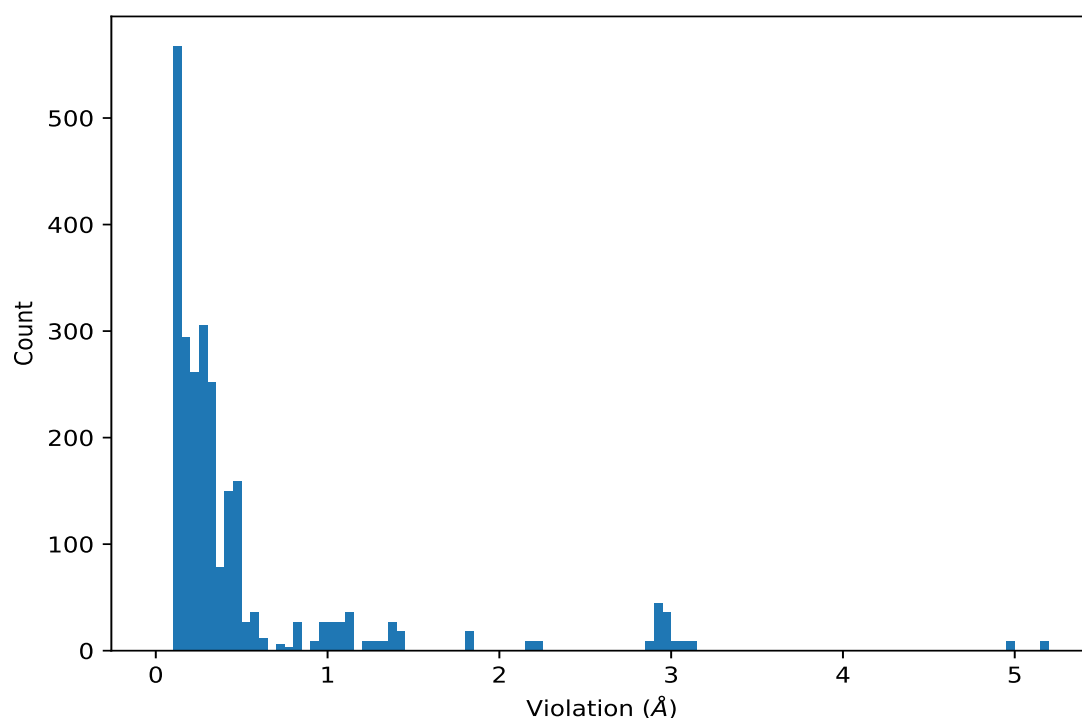
| Key     | Atom-1           | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|------------------|----------------|---------------------|----------|---------------------|------------|
| (1,252) | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA | 3                   | 0.22     | 0.09                | 0.16       |
| (1,353) | 1:237:C:TRP:H    | 1:234:C:SER:HA | 3                   | 0.22     | 0.07                | 0.23       |
| (1,5)   | 1:212:C:SER:H    | 1:211:C:LEU:H  | 3                   | 0.21     | 0.06                | 0.21       |
| (1,124) | 1:212:C:SER:H    | 1:211:C:LEU:H  | 3                   | 0.21     | 0.06                | 0.21       |
| (1,243) | 1:212:C:SER:H    | 1:211:C:LEU:H  | 3                   | 0.21     | 0.06                | 0.21       |
| (1,78)  | 1:228:C:ALA:H    | 1:227:C:VAL:HA | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,197) | 1:228:C:ALA:H    | 1:227:C:VAL:HA | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,316) | 1:228:C:ALA:H    | 1:227:C:VAL:HA | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,118) | 1:238:C:LYS:H    | 1:239:C:LYS:H  | 2                   | 0.2      | 0.06                | 0.2        |
| (1,119) | 1:239:C:LYS:H    | 1:238:C:LYS:H  | 2                   | 0.2      | 0.06                | 0.2        |
| (1,237) | 1:238:C:LYS:H    | 1:239:C:LYS:H  | 2                   | 0.2      | 0.06                | 0.2        |
| (1,238) | 1:239:C:LYS:H    | 1:238:C:LYS:H  | 2                   | 0.2      | 0.06                | 0.2        |
| (1,356) | 1:238:C:LYS:H    | 1:239:C:LYS:H  | 2                   | 0.2      | 0.06                | 0.2        |
| (1,357) | 1:239:C:LYS:H    | 1:238:C:LYS:H  | 2                   | 0.2      | 0.06                | 0.2        |
| (1,16)  | 1:214:C:ILE:HG21 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,16)  | 1:214:C:ILE:HG22 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,16)  | 1:214:C:ILE:HG23 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,135) | 1:214:C:ILE:HG21 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,135) | 1:214:C:ILE:HG22 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,135) | 1:214:C:ILE:HG23 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,254) | 1:214:C:ILE:HG21 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,254) | 1:214:C:ILE:HG22 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,254) | 1:214:C:ILE:HG23 | 1:218:C:VAL:H  | 2                   | 0.19     | 0.04                | 0.19       |
| (1,1)   | 1:211:C:LEU:H    | 1:210:C:SER:HA | 2                   | 0.15     | 0.03                | 0.15       |
| (1,120) | 1:211:C:LEU:H    | 1:210:C:SER:HA | 2                   | 0.15     | 0.03                | 0.15       |
| (1,239) | 1:211:C:LEU:H    | 1:210:C:SER:HA | 2                   | 0.15     | 0.03                | 0.15       |
| (1,102) | 1:233:C:LYS:H    | 1:230:C:PHE:HA | 2                   | 0.14     | 0.03                | 0.14       |
| (1,221) | 1:233:C:LYS:H    | 1:230:C:PHE:HA | 2                   | 0.14     | 0.03                | 0.14       |
| (1,340) | 1:233:C:LYS:H    | 1:230:C:PHE:HA | 2                   | 0.14     | 0.03                | 0.14       |

<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) |
|---------|------------------|----------------|----------|---------------|
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 8        | 5.17          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 13       | 4.97          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 13       | 4.97          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 13       | 4.97          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 13       | 4.97          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 13       | 4.97          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 13       | 4.97          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 13       | 4.97          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 13       | 4.97          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 13       | 4.97          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 12       | 3.11          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 14       | 3.09          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 3        | 3.0           |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 4        | 2.99          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 9        | 2.97          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 9        | 2.97          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 9        | 2.97          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 9        | 2.97          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 9        | 2.97          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 9        | 2.97          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 7        | 2.97          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 9        | 2.97          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 9        | 2.97          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 9        | 2.97          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 2        | 2.96          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 1        | 2.94          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA | 10       | 2.94          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA | 5        | 2.93          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 5        | 2.93          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 5        | 2.93          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 5        | 2.93          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 5        | 2.93          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 5        | 2.93          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 5        | 2.93          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 5        | 2.93          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 5        | 2.93          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 6        | 2.91          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 11       | 2.91          |
| (1,369) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,369) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,369) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,368) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,368) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,368) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,367) | 1:223:C:VAL:HG21 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,367) | 1:223:C:VAL:HG22 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,367) | 1:223:C:VAL:HG23 | 1:218:C:VAL:HA   | 15       | 2.88          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 13       | 2.2           |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 13       | 2.2           |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 13       | 2.2           |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 13       | 2.2           |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 13       | 2.2           |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 13       | 2.2           |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 13       | 2.2           |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 13       | 2.2           |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 13       | 2.2           |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 8        | 2.19          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 8        | 2.19          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 8        | 2.19          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 8        | 2.19          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 8        | 2.19          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 8        | 2.19          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 8        | 2.19          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 8        | 2.19          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 8        | 2.19          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 13       | 1.84          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA   | 8        | 1.82          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 4        | 1.43          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 14       | 1.42          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 14       | 1.42          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 14       | 1.42          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 14       | 1.42          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 14       | 1.42          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 14       | 1.42          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 14       | 1.42          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 14       | 1.42          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 14       | 1.42          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 11       | 1.38          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 10       | 1.36          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 13       | 1.35          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 13       | 1.35          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 13       | 1.35          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 13       | 1.35          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 13       | 1.35          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 13       | 1.35          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 13       | 1.35          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 13       | 1.35          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 13       | 1.35          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 3        | 1.3           |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 8        | 1.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 8        | 1.27          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 8        | 1.27          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 8        | 1.27          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 8        | 1.27          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 8        | 1.27          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 8        | 1.27          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 8        | 1.27          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 8        | 1.27          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 13       | 1.23          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 3        | 1.14          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 3        | 1.14          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 3        | 1.14          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 3        | 1.14          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 3        | 1.14          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 3        | 1.14          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 3        | 1.14          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 3        | 1.14          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 3        | 1.14          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 12       | 1.12          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 12       | 1.12          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 12       | 1.12          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 15       | 1.12          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 15       | 1.12          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 15       | 1.12          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 12       | 1.12          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 12       | 1.12          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 12       | 1.12          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 15       | 1.12          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 15       | 1.12          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 15       | 1.12          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 12       | 1.12          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 12       | 1.12          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 12       | 1.12          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 15       | 1.12          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 15       | 1.12          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 15       | 1.12          |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 11       | 1.11          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 8        | 1.09          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 8        | 1.09          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 8        | 1.09          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 14       | 1.09          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 14       | 1.09          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 14       | 1.09          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 8        | 1.09          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 8        | 1.09          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 8        | 1.09          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 14       | 1.09          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 14       | 1.09          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 14       | 1.09          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 8        | 1.09          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 8        | 1.09          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 8        | 1.09          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 14       | 1.09          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 14       | 1.09          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 14       | 1.09          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 15       | 1.05          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 1        | 1.04          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 1        | 1.04          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 1        | 1.04          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 1        | 1.04          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 1        | 1.04          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 1        | 1.04          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 1        | 1.04          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 1        | 1.04          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 1        | 1.04          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 5        | 1.03          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 5        | 1.03          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 5        | 1.03          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 5        | 1.03          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 5        | 1.03          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 5        | 1.03          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 5        | 1.03          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 5        | 1.03          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 5        | 1.03          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 7        | 1.02          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 7        | 1.02          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 7        | 1.02          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 7        | 1.02          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 7        | 1.02          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 7        | 1.02          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 7        | 1.02          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 7        | 1.02          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 7        | 1.02          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 7        | 0.99          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 12       | 0.98          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 1        | 0.97          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 1        | 0.97          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 1        | 0.97          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 1        | 0.97          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 1        | 0.97          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 1        | 0.97          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 1        | 0.97          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 1        | 0.97          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 1        | 0.97          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 10       | 0.94          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 10       | 0.94          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 10       | 0.94          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 10       | 0.94          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 10       | 0.94          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 10       | 0.94          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 10       | 0.94          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 10       | 0.94          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 10       | 0.94          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 5        | 0.83          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 2        | 0.82          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 9        | 0.8           |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 9        | 0.8           |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 9        | 0.8           |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 9        | 0.8           |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG   | 9        | 0.8           |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG   | 9        | 0.8           |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG   | 9        | 0.8           |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG  | 9        | 0.8           |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG  | 9        | 0.8           |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 7        | 0.78          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 7        | 0.78          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 7        | 0.78          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 5        | 0.72          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 11       | 0.72          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 5        | 0.72          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 11       | 0.72          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 5        | 0.72          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 11       | 0.72          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 8        | 0.64          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 8        | 0.64          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 8        | 0.64          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 11       | 0.63          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 11       | 0.63          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 11       | 0.63          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 11       | 0.63          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 11       | 0.63          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 11       | 0.63          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 1        | 0.62          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 1        | 0.62          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 1        | 0.62          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 8        | 0.58          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 13       | 0.58          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 8        | 0.58          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 13       | 0.58          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 8        | 0.58          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 13       | 0.58          |
| (1,253) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 12       | 0.57          |
| (1,253) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,253) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 12       | 0.57          |
| (1,253) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,253) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 12       | 0.57          |
| (1,253) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,134) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 12       | 0.57          |
| (1,134) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,134) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 12       | 0.57          |
| (1,134) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,134) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 12       | 0.57          |
| (1,134) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,15)  | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 12       | 0.57          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,15)  | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,15)  | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 12       | 0.57          |
| (1,15)  | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,15)  | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 12       | 0.57          |
| (1,15)  | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 12       | 0.57          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 9        | 0.56          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 9        | 0.56          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 9        | 0.56          |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 8        | 0.55          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 12       | 0.54          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 12       | 0.54          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 12       | 0.54          |
| (1,330) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 3        | 0.53          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 15       | 0.53          |
| (1,211) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 3        | 0.53          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 15       | 0.53          |
| (1,92)  | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 3        | 0.53          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 15       | 0.53          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 13       | 0.52          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 10       | 0.52          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 10       | 0.52          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 13       | 0.52          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 10       | 0.52          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 10       | 0.52          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 13       | 0.52          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 10       | 0.52          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 10       | 0.52          |
| (1,330) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 11       | 0.51          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 14       | 0.51          |
| (1,211) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 11       | 0.51          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 14       | 0.51          |
| (1,92)  | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 11       | 0.51          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 14       | 0.51          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 13       | 0.5           |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 13       | 0.5           |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 13       | 0.5           |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 6        | 0.49          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 9        | 0.49          |
| (1,330) | 1:231:C:VAL:H    | 1:228:C:ALA:HA | 6        | 0.49          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA | 2        | 0.49          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA | 7        | 0.49          |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,211) | 1:231:C:VAL:H    | 1:228:C:ALA:HA | 6        | 0.49          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA | 2        | 0.49          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA | 7        | 0.49          |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,92)  | 1:231:C:VAL:H    | 1:228:C:ALA:HA | 6        | 0.49          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA | 2        | 0.49          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA | 7        | 0.49          |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H  | 1        | 0.49          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 2        | 0.48          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 2        | 0.48          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 2        | 0.48          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 2        | 0.48          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 2        | 0.48          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 2        | 0.48          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 2        | 0.48          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 2        | 0.48          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 2        | 0.48          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 8        | 0.48          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 15       | 0.48          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 8        | 0.48          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 15       | 0.48          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 8        | 0.48          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA | 15       | 0.48          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 5        | 0.47          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 11       | 0.47          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 5        | 0.47          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 11       | 0.47          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA | 5        | 0.47          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA | 11       | 0.47          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 10       | 0.46          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 10       | 0.46          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 10       | 0.46          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 10       | 0.46          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 10       | 0.46          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 10       | 0.46          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 1        | 0.46          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 5        | 0.46          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 10       | 0.46          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 10       | 0.46          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 10       | 0.46          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 15       | 0.46          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 10       | 0.46          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 14       | 0.46          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 7        | 0.46          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 12       | 0.46          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA | 11       | 0.46          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 15       | 0.46          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 10       | 0.46          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 14       | 0.46          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 7        | 0.46          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 12       | 0.46          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA | 11       | 0.46          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 15       | 0.46          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 10       | 0.46          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 14       | 0.46          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 7        | 0.46          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 12       | 0.46          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA | 11       | 0.46          |
| (1,375) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,375) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,375) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,374) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,374) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,374) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,373) | 1:226:C:ILE:HD11 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,373) | 1:226:C:ILE:HD12 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,373) | 1:226:C:ILE:HD13 | 1:225:C:LEU:HG | 6        | 0.45          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 4        | 0.45          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 4        | 0.45          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 4        | 0.45          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 4        | 0.45          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 4        | 0.45          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 4        | 0.45          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 4        | 0.45          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 4        | 0.45          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 4        | 0.45          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 7        | 0.45          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 12       | 0.45          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 15       | 0.45          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 9        | 0.45          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 7        | 0.45          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 12       | 0.45          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 14       | 0.45          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 9        | 0.45          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 7        | 0.45          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 12       | 0.45          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 14       | 0.45          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 9        | 0.45          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA | 7        | 0.45          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA | 12       | 0.45          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 14       | 0.45          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,372) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 14       | 0.44          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,372) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 14       | 0.44          |
| (1,372) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 14       | 0.44          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,371) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 14       | 0.44          |
| (1,371) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 14       | 0.44          |
| (1,371) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 14       | 0.44          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 3        | 0.44          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 11       | 0.44          |
| (1,370) | 1:223:C:VAL:HG21 | 1:222:C:ALA:HA | 14       | 0.44          |
| (1,370) | 1:223:C:VAL:HG22 | 1:222:C:ALA:HA | 14       | 0.44          |
| (1,370) | 1:223:C:VAL:HG23 | 1:222:C:ALA:HA | 14       | 0.44          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 12       | 0.44          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA | 14       | 0.44          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 13       | 0.44          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 13       | 0.44          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA | 13       | 0.44          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA | 5        | 0.44          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 4        | 0.44          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 8        | 0.44          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 1        | 0.44          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 12       | 0.44          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA | 14       | 0.44          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 13       | 0.44          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 13       | 0.44          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA | 13       | 0.44          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA | 5        | 0.44          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 4        | 0.44          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 8        | 0.44          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 1        | 0.44          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 12       | 0.44          |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA | 14       | 0.44          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 13       | 0.44          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 13       | 0.44          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 13       | 0.44          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 5        | 0.44          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 4        | 0.44          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 8        | 0.44          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 1        | 0.44          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 6        | 0.43          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 5        | 0.43          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 7        | 0.43          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 9        | 0.43          |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 13       | 0.43          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 3        | 0.43          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 10       | 0.43          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 6        | 0.43          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 5        | 0.43          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 7        | 0.43          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 9        | 0.43          |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 13       | 0.43          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 3        | 0.43          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 10       | 0.43          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 6        | 0.43          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 5        | 0.43          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 7        | 0.43          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 9        | 0.43          |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 13       | 0.43          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 3        | 0.43          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 10       | 0.43          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 9        | 0.42          |
| (1,314) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 7        | 0.42          |
| (1,314) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 7        | 0.42          |
| (1,314) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 7        | 0.42          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 13       | 0.42          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 7        | 0.42          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 7        | 0.42          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 2        | 0.42          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 9        | 0.42          |
| (1,195) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 7        | 0.42          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,195) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 7        | 0.42          |
| (1,195) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 7        | 0.42          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 13       | 0.42          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 7        | 0.42          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 7        | 0.42          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 2        | 0.42          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 9        | 0.42          |
| (1,76)  | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 7        | 0.42          |
| (1,76)  | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 7        | 0.42          |
| (1,76)  | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 7        | 0.42          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 13       | 0.42          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 11       | 0.42          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 11       | 0.42          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 7        | 0.42          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 7        | 0.42          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 2        | 0.42          |
| (1,355) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA  | 8        | 0.41          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 13       | 0.41          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 13       | 0.41          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 14       | 0.41          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 15       | 0.41          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 13       | 0.41          |
| (1,236) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA  | 8        | 0.41          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 13       | 0.41          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 13       | 0.41          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 14       | 0.41          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 15       | 0.41          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 13       | 0.41          |
| (1,117) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA  | 8        | 0.41          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 13       | 0.41          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 13       | 0.41          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 14       | 0.41          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA   | 15       | 0.41          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 13       | 0.41          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 4        | 0.4           |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 4        | 0.4           |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 4        | 0.4           |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 4        | 0.4           |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 4        | 0.4           |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 4        | 0.4           |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 4        | 0.4           |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 4        | 0.4           |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 4        | 0.4           |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 8        | 0.4           |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 4        | 0.4           |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 8        | 0.4           |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 4        | 0.4           |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 8        | 0.4           |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 4        | 0.4           |
| (1,314) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,314) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,314) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 6        | 0.39          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA   | 10       | 0.39          |
| (1,195) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,195) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,195) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 6        | 0.39          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA   | 10       | 0.39          |
| (1,76)  | 1:227:C:VAL:HG21 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,76)  | 1:227:C:VAL:HG22 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,76)  | 1:227:C:VAL:HG23 | 1:231:C:VAL:H    | 5        | 0.39          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 6        | 0.39          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA   | 10       | 0.39          |
| (1,314) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H    | 2        | 0.38          |
| (1,314) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H    | 2        | 0.38          |
| (1,314) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H    | 2        | 0.38          |
| (1,313) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA   | 3        | 0.38          |
| (1,313) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA   | 3        | 0.38          |
| (1,313) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA   | 3        | 0.38          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA   | 1        | 0.38          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 6        | 0.38          |
| (1,195) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H    | 2        | 0.38          |
| (1,195) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H    | 2        | 0.38          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,195) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H  | 2        | 0.38          |
| (1,194) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA | 3        | 0.38          |
| (1,194) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA | 3        | 0.38          |
| (1,194) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA | 3        | 0.38          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 1        | 0.38          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA | 6        | 0.38          |
| (1,76)  | 1:227:C:VAL:HG21 | 1:231:C:VAL:H  | 2        | 0.38          |
| (1,76)  | 1:227:C:VAL:HG22 | 1:231:C:VAL:H  | 2        | 0.38          |
| (1,76)  | 1:227:C:VAL:HG23 | 1:231:C:VAL:H  | 2        | 0.38          |
| (1,75)  | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA | 3        | 0.38          |
| (1,75)  | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA | 3        | 0.38          |
| (1,75)  | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA | 3        | 0.38          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA | 1        | 0.38          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA | 6        | 0.38          |
| (1,355) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA | 4        | 0.37          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 8        | 0.37          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 3        | 0.37          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 6        | 0.37          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 8        | 0.37          |
| (1,236) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA | 4        | 0.37          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 8        | 0.37          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 3        | 0.37          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 6        | 0.37          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 8        | 0.37          |
| (1,117) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA | 4        | 0.37          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 8        | 0.37          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 3        | 0.37          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA | 6        | 0.37          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 8        | 0.37          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 8        | 0.36          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 3        | 0.36          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 4        | 0.36          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 6        | 0.36          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 15       | 0.36          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA | 8        | 0.36          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 3        | 0.36          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 4        | 0.36          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 6        | 0.36          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 15       | 0.36          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA | 15       | 0.36          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA | 8        | 0.36          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 3        | 0.36          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA | 4        | 0.36          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 6        | 0.36          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 15       | 0.36          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 4        | 0.35          |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA | 6        | 0.35          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 7        | 0.35          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 13       | 0.35          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 2        | 0.35          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA | 6        | 0.35          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA | 4        | 0.35          |
| (1,252) | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,252) | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,252) | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA | 8        | 0.35          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 4        | 0.35          |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA | 6        | 0.35          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 7        | 0.35          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 13       | 0.35          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 2        | 0.35          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA | 6        | 0.35          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA | 4        | 0.35          |
| (1,133) | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,133) | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,133) | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA | 8        | 0.35          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA | 4        | 0.35          |
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA | 6        | 0.35          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 7        | 0.35          |

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| Key     | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|---------|------------------|----------------|----------|---------------|
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 13       | 0.35          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA | 2        | 0.35          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA | 3        | 0.35          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA | 6        | 0.35          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA | 4        | 0.35          |
| (1,14)  | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,14)  | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,14)  | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA | 5        | 0.35          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA | 8        | 0.35          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 3        | 0.34          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 2        | 0.34          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 5        | 0.34          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 3        | 0.34          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 4        | 0.34          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 5        | 0.34          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA | 6        | 0.34          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA | 9        | 0.34          |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H  | 15       | 0.34          |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H  | 15       | 0.34          |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H  | 15       | 0.34          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 3        | 0.34          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 2        | 0.34          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 5        | 0.34          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 3        | 0.34          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 4        | 0.34          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 5        | 0.34          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA | 6        | 0.34          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA | 9        | 0.34          |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H  | 15       | 0.34          |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H  | 15       | 0.34          |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H  | 15       | 0.34          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA | 3        | 0.34          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 2        | 0.34          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA | 5        | 0.34          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 3        | 0.34          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 4        | 0.34          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA | 5        | 0.34          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA | 6        | 0.34          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA | 9        | 0.34          |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H  | 15       | 0.34          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 15       | 0.34          |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 15       | 0.34          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 1        | 0.33          |
| (1,314) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,314) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,314) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,314) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,314) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,314) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 12       | 0.33          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 14       | 0.33          |
| (1,269) | 1:218:C:VAL:H    | 1:214:C:ILE:HA  | 13       | 0.33          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 12       | 0.33          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 12       | 0.33          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 3        | 0.33          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 1        | 0.33          |
| (1,195) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,195) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,195) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,195) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,195) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,195) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 12       | 0.33          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 14       | 0.33          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,150) | 1:218:C:VAL:H    | 1:214:C:ILE:HA  | 13       | 0.33          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 12       | 0.33          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 12       | 0.33          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 3        | 0.33          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 1        | 0.33          |
| (1,76)  | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,76)  | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,76)  | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 4        | 0.33          |
| (1,76)  | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,76)  | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,76)  | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 11       | 0.33          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 4        | 0.33          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 10       | 0.33          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 12       | 0.33          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 14       | 0.33          |
| (1,31)  | 1:218:C:VAL:H    | 1:214:C:ILE:HA  | 13       | 0.33          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 8        | 0.33          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 8        | 0.33          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 12       | 0.33          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 12       | 0.33          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 3        | 0.33          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 12       | 0.32          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 2        | 0.32          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 7        | 0.32          |
| (1,264) | 1:216:C:ILE:HG21 | 1:220:C:VAL:HB  | 13       | 0.32          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,264) | 1:216:C:ILE:HG22 | 1:220:C:VAL:HB  | 13       | 0.32          |
| (1,264) | 1:216:C:ILE:HG23 | 1:220:C:VAL:HB  | 13       | 0.32          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 1        | 0.32          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 1        | 0.32          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 13       | 0.32          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 15       | 0.32          |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 12       | 0.32          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 2        | 0.32          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 7        | 0.32          |
| (1,145) | 1:216:C:ILE:HG21 | 1:220:C:VAL:HB  | 13       | 0.32          |
| (1,145) | 1:216:C:ILE:HG22 | 1:220:C:VAL:HB  | 13       | 0.32          |
| (1,145) | 1:216:C:ILE:HG23 | 1:220:C:VAL:HB  | 13       | 0.32          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 1        | 0.32          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 1        | 0.32          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 13       | 0.32          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 15       | 0.32          |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 12       | 0.32          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 12       | 0.32          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 2        | 0.32          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 7        | 0.32          |
| (1,26)  | 1:216:C:ILE:HG21 | 1:220:C:VAL:HB  | 13       | 0.32          |
| (1,26)  | 1:216:C:ILE:HG22 | 1:220:C:VAL:HB  | 13       | 0.32          |
| (1,26)  | 1:216:C:ILE:HG23 | 1:220:C:VAL:HB  | 13       | 0.32          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 12       | 0.32          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 12       | 0.32          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 1        | 0.32          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 1        | 0.32          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 13       | 0.32          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 15       | 0.32          |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 10       | 0.32          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 6        | 0.31          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 9        | 0.31          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 10       | 0.31          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 4        | 0.31          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 15       | 0.31          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 5        | 0.31          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 6        | 0.31          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 9        | 0.31          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 10       | 0.31          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 4        | 0.31          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 15       | 0.31          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 5        | 0.31          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 6        | 0.31          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 9        | 0.31          |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 10       | 0.31          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 4        | 0.31          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 15       | 0.31          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 5        | 0.31          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 5        | 0.31          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 5        | 0.31          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 7        | 0.3           |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 7        | 0.3           |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 7        | 0.3           |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 8        | 0.3           |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 4        | 0.3           |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 7        | 0.3           |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 7        | 0.3           |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 7        | 0.3           |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 8        | 0.3           |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 4        | 0.3           |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 13       | 0.3           |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 13       | 0.3           |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 1        | 0.3           |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 7        | 0.3           |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 7        | 0.3           |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 7        | 0.3           |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 11       | 0.3           |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 14       | 0.3           |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 8        | 0.3           |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 4        | 0.3           |
| (1,353) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 8        | 0.29          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 2        | 0.29          |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,315) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 8        | 0.29          |
| (1,314) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,314) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,314) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 1        | 0.29          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 5        | 0.29          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 5        | 0.29          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 5        | 0.29          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 2        | 0.29          |
| (1,289) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 9        | 0.29          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 8        | 0.29          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 8        | 0.29          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 15       | 0.29          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 15       | 0.29          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 9        | 0.29          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 15       | 0.29          |
| (1,234) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 8        | 0.29          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 2        | 0.29          |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,196) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 8        | 0.29          |
| (1,195) | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,195) | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,195) | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 1        | 0.29          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 5        | 0.29          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 5        | 0.29          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 5        | 0.29          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 2        | 0.29          |
| (1,170) | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 9        | 0.29          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 8        | 0.29          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 8        | 0.29          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 15       | 0.29          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 15       | 0.29          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 9        | 0.29          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 15       | 0.29          |
| (1,115) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 8        | 0.29          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 2        | 0.29          |
| (1,86)  | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,86)  | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,86)  | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 6        | 0.29          |
| (1,77)  | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 8        | 0.29          |
| (1,76)  | 1:227:C:VAL:HG21 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,76)  | 1:227:C:VAL:HG22 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,76)  | 1:227:C:VAL:HG23 | 1:231:C:VAL:H   | 6        | 0.29          |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 1        | 0.29          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 5        | 0.29          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 5        | 0.29          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 5        | 0.29          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 2        | 0.29          |
| (1,51)  | 1:222:C:ALA:H    | 1:219:C:THR:HA  | 9        | 0.29          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 8        | 0.29          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 8        | 0.29          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 15       | 0.29          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 15       | 0.29          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 9        | 0.29          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 15       | 0.29          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 6        | 0.28          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 12       | 0.28          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 9        | 0.28          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 9        | 0.28          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 11       | 0.28          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 9        | 0.28          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 9        | 0.28          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 14       | 0.28          |
| (1,243) | 1:212:C:SER:H    | 1:211:C:LEU:H   | 14       | 0.28          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 6        | 0.28          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 12       | 0.28          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 9        | 0.28          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 9        | 0.28          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 11       | 0.28          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 9        | 0.28          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 9        | 0.28          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 14       | 0.28          |
| (1,124) | 1:212:C:SER:H    | 1:211:C:LEU:H   | 14       | 0.28          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 6        | 0.28          |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 12       | 0.28          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 9        | 0.28          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 9        | 0.28          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 11       | 0.28          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 9        | 0.28          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 9        | 0.28          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 14       | 0.28          |
| (1,5)   | 1:212:C:SER:H    | 1:211:C:LEU:H   | 14       | 0.28          |
| (1,330) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 4        | 0.27          |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 4        | 0.27          |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 4        | 0.27          |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 4        | 0.27          |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 4        | 0.27          |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 4        | 0.27          |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 4        | 0.27          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 10       | 0.27          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 11       | 0.27          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 14       | 0.27          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA   | 9        | 0.27          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 1        | 0.27          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 10       | 0.27          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA   | 13       | 0.27          |
| (1,211) | 1:231:C:VAL:H    | 1:228:C:ALA:HA   | 4        | 0.27          |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1  | 4        | 0.27          |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2  | 4        | 0.27          |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1  | 4        | 0.27          |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2  | 4        | 0.27          |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1  | 4        | 0.27          |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2  | 4        | 0.27          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 10       | 0.27          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 11       | 0.27          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 14       | 0.27          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA   | 9        | 0.27          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 1        | 0.27          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 10       | 0.27          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA   | 13       | 0.27          |
| (1,92)  | 1:231:C:VAL:H    | 1:228:C:ALA:HA   | 4        | 0.27          |
| (1,70)  | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1  | 4        | 0.27          |
| (1,70)  | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2  | 4        | 0.27          |
| (1,70)  | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1  | 4        | 0.27          |
| (1,70)  | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2  | 4        | 0.27          |
| (1,70)  | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1  | 4        | 0.27          |
| (1,70)  | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2  | 4        | 0.27          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 10       | 0.27          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 11       | 0.27          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 14       | 0.27          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA   | 9        | 0.27          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 1        | 0.27          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA   | 10       | 0.27          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA   | 13       | 0.27          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 6        | 0.26          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 6        | 0.26          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 6        | 0.26          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 6        | 0.26          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 6        | 0.26          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 6        | 0.26          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 6        | 0.26          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 6        | 0.26          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 6        | 0.26          |
| (1,357) | 1:239:C:LYS:H    | 1:238:C:LYS:H    | 3        | 0.26          |
| (1,356) | 1:238:C:LYS:H    | 1:239:C:LYS:H    | 3        | 0.26          |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 11       | 0.26          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA   | 7        | 0.26          |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA   | 15       | 0.26          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 12       | 0.26          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 12       | 0.26          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 14       | 0.26          |
| (1,238) | 1:239:C:LYS:H    | 1:238:C:LYS:H    | 3        | 0.26          |
| (1,237) | 1:238:C:LYS:H    | 1:239:C:LYS:H    | 3        | 0.26          |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 11       | 0.26          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA   | 7        | 0.26          |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA   | 15       | 0.26          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 12       | 0.26          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 12       | 0.26          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 14       | 0.26          |
| (1,119) | 1:239:C:LYS:H    | 1:238:C:LYS:H    | 3        | 0.26          |
| (1,118) | 1:238:C:LYS:H    | 1:239:C:LYS:H    | 3        | 0.26          |
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 11       | 0.26          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA   | 7        | 0.26          |
| (1,86)  | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,86)  | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,86)  | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 3        | 0.26          |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA   | 15       | 0.26          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 12       | 0.26          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 12       | 0.26          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 14       | 0.26          |
| (1,330) | 1:231:C:VAL:H    | 1:228:C:ALA:HA   | 15       | 0.25          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA   | 11       | 0.25          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2  | 10       | 0.25          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3  | 10       | 0.25          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2  | 10       | 0.25          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3  | 10       | 0.25          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2  | 10       | 0.25          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 10       | 0.25          |
| (1,313) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 10       | 0.25          |
| (1,313) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 10       | 0.25          |
| (1,313) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 10       | 0.25          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 3        | 0.25          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 1        | 0.25          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 4        | 0.25          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 3        | 0.25          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 8        | 0.25          |
| (1,270) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 13       | 0.25          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 6        | 0.25          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 6        | 0.25          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 6        | 0.25          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 6        | 0.25          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 6        | 0.25          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 6        | 0.25          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 3        | 0.25          |
| (1,211) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 15       | 0.25          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA  | 11       | 0.25          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 10       | 0.25          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 10       | 0.25          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 10       | 0.25          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 10       | 0.25          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 10       | 0.25          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 10       | 0.25          |
| (1,194) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 10       | 0.25          |
| (1,194) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 10       | 0.25          |
| (1,194) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 10       | 0.25          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 3        | 0.25          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 1        | 0.25          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 4        | 0.25          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 3        | 0.25          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 8        | 0.25          |
| (1,151) | 1:218:C:VAL:H    | 1:215:C:ILE:HA  | 13       | 0.25          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 6        | 0.25          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 6        | 0.25          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 6        | 0.25          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 6        | 0.25          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 6        | 0.25          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 6        | 0.25          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 3        | 0.25          |
| (1,92)  | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 15       | 0.25          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA   | 11       | 0.25          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2  | 10       | 0.25          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3  | 10       | 0.25          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2  | 10       | 0.25          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3  | 10       | 0.25          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2  | 10       | 0.25          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3  | 10       | 0.25          |
| (1,75)  | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA   | 10       | 0.25          |
| (1,75)  | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA   | 10       | 0.25          |
| (1,75)  | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA   | 10       | 0.25          |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA   | 3        | 0.25          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 1        | 0.25          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 4        | 0.25          |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 3        | 0.25          |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 8        | 0.25          |
| (1,32)  | 1:218:C:VAL:H    | 1:215:C:ILE:HA   | 13       | 0.25          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2  | 6        | 0.25          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3  | 6        | 0.25          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2  | 6        | 0.25          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3  | 6        | 0.25          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2  | 6        | 0.25          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3  | 6        | 0.25          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 3        | 0.25          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 14       | 0.24          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 14       | 0.24          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 14       | 0.24          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 14       | 0.24          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 14       | 0.24          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 14       | 0.24          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 14       | 0.24          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 14       | 0.24          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 14       | 0.24          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 3        | 0.24          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 12       | 0.24          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 11       | 0.24          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 15       | 0.24          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA   | 6        | 0.24          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA   | 6        | 0.24          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA   | 6        | 0.24          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2  | 2        | 0.24          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3  | 2        | 0.24          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 5        | 0.24          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 3        | 0.24          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 12       | 0.24          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 11       | 0.24          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 15       | 0.24          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 6        | 0.24          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 6        | 0.24          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 6        | 0.24          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 2        | 0.24          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 2        | 0.24          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 5        | 0.24          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 3        | 0.24          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 12       | 0.24          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 11       | 0.24          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 15       | 0.24          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 6        | 0.24          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 6        | 0.24          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 6        | 0.24          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 2        | 0.24          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 2        | 0.24          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 5        | 0.24          |
| (1,353) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 11       | 0.23          |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 4        | 0.23          |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 4        | 0.23          |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 4        | 0.23          |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 9        | 0.23          |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 9        | 0.23          |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 9        | 0.23          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 1        | 0.23          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA  | 8        | 0.23          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 9        | 0.23          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 9        | 0.23          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 9        | 0.23          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 8        | 0.23          |
| (1,254) | 1:214:C:ILE:HG21 | 1:218:C:VAL:H   | 12       | 0.23          |
| (1,254) | 1:214:C:ILE:HG22 | 1:218:C:VAL:H   | 12       | 0.23          |
| (1,254) | 1:214:C:ILE:HG23 | 1:218:C:VAL:H   | 12       | 0.23          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 5        | 0.23          |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 14       | 0.23          |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 14       | 0.23          |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 14       | 0.23          |
| (1,234) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 11       | 0.23          |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 4        | 0.23          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 4        | 0.23          |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 4        | 0.23          |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 9        | 0.23          |
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 9        | 0.23          |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 9        | 0.23          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 1        | 0.23          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 8        | 0.23          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA   | 9        | 0.23          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA   | 9        | 0.23          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA   | 9        | 0.23          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 8        | 0.23          |
| (1,135) | 1:214:C:ILE:HG21 | 1:218:C:VAL:H    | 12       | 0.23          |
| (1,135) | 1:214:C:ILE:HG22 | 1:218:C:VAL:H    | 12       | 0.23          |
| (1,135) | 1:214:C:ILE:HG23 | 1:218:C:VAL:H    | 12       | 0.23          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 5        | 0.23          |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 14       | 0.23          |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 14       | 0.23          |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 14       | 0.23          |
| (1,115) | 1:237:C:TRP:H    | 1:234:C:SER:HA   | 11       | 0.23          |
| (1,86)  | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 4        | 0.23          |
| (1,86)  | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 4        | 0.23          |
| (1,86)  | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 4        | 0.23          |
| (1,86)  | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 9        | 0.23          |
| (1,86)  | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 9        | 0.23          |
| (1,86)  | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 9        | 0.23          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 1        | 0.23          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 8        | 0.23          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA   | 9        | 0.23          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA   | 9        | 0.23          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA   | 9        | 0.23          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 8        | 0.23          |
| (1,16)  | 1:214:C:ILE:HG21 | 1:218:C:VAL:H    | 12       | 0.23          |
| (1,16)  | 1:214:C:ILE:HG22 | 1:218:C:VAL:H    | 12       | 0.23          |
| (1,16)  | 1:214:C:ILE:HG23 | 1:218:C:VAL:H    | 12       | 0.23          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 5        | 0.23          |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 14       | 0.23          |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 14       | 0.23          |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 14       | 0.23          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 9        | 0.22          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 9        | 0.22          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 9        | 0.22          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 9        | 0.22          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 9        | 0.22          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 9        | 0.22          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 9        | 0.22          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 9        | 0.22          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 9        | 0.22          |
| (1,326) | 1:230:C:PHE:H    | 1:227:C:VAL:HA   | 5        | 0.22          |
| (1,305) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 15       | 0.22          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 3        | 0.22          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA   | 7        | 0.22          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2  | 4        | 0.22          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3  | 4        | 0.22          |
| (1,207) | 1:230:C:PHE:H    | 1:227:C:VAL:HA   | 5        | 0.22          |
| (1,186) | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 15       | 0.22          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 3        | 0.22          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA   | 7        | 0.22          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2  | 4        | 0.22          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3  | 4        | 0.22          |
| (1,88)  | 1:230:C:PHE:H    | 1:227:C:VAL:HA   | 5        | 0.22          |
| (1,67)  | 1:226:C:ILE:H    | 1:223:C:VAL:HA   | 15       | 0.22          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 3        | 0.22          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA   | 7        | 0.22          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2  | 4        | 0.22          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3  | 4        | 0.22          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 12       | 0.21          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 12       | 0.21          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 12       | 0.21          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 12       | 0.21          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 12       | 0.21          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 12       | 0.21          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 12       | 0.21          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 12       | 0.21          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 12       | 0.21          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 14       | 0.21          |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 9        | 0.21          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 10       | 0.21          |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA   | 11       | 0.21          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 6        | 0.21          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 3        | 0.21          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 9        | 0.21          |
| (1,243) | 1:212:C:SER:H    | 1:211:C:LEU:H    | 13       | 0.21          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA   | 1        | 0.21          |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 12       | 0.21          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 12       | 0.21          |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 12       | 0.21          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 14       | 0.21          |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 9        | 0.21          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 10       | 0.21          |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA   | 11       | 0.21          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 6        | 0.21          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 3        | 0.21          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 9        | 0.21          |
| (1,124) | 1:212:C:SER:H    | 1:211:C:LEU:H    | 13       | 0.21          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA   | 1        | 0.21          |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 12       | 0.21          |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 12       | 0.21          |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 12       | 0.21          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 14       | 0.21          |
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 9        | 0.21          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 10       | 0.21          |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA   | 11       | 0.21          |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 6        | 0.21          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 3        | 0.21          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 9        | 0.21          |
| (1,5)   | 1:212:C:SER:H    | 1:211:C:LEU:H    | 13       | 0.21          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA   | 1        | 0.21          |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 12       | 0.21          |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 12       | 0.21          |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 12       | 0.21          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 2        | 0.2           |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 2        | 0.2           |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 2        | 0.2           |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 2        | 0.2           |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 2        | 0.2           |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 2        | 0.2           |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 2        | 0.2           |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 2        | 0.2           |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 2        | 0.2           |
| (1,355) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA   | 7        | 0.2           |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 15       | 0.2           |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 15       | 0.2           |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 15       | 0.2           |
| (1,313) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA   | 15       | 0.2           |
| (1,313) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA   | 15       | 0.2           |
| (1,313) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA   | 15       | 0.2           |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 14       | 0.2           |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 14       | 0.2           |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 11       | 0.2           |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 14       | 0.2           |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 14       | 0.2           |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 14       | 0.2           |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 7        | 0.2           |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 11       | 0.2           |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,236) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA  | 7        | 0.2           |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 15       | 0.2           |
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 15       | 0.2           |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 15       | 0.2           |
| (1,194) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 15       | 0.2           |
| (1,194) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 15       | 0.2           |
| (1,194) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 15       | 0.2           |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 14       | 0.2           |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 14       | 0.2           |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 11       | 0.2           |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 14       | 0.2           |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 14       | 0.2           |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 14       | 0.2           |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 7        | 0.2           |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 11       | 0.2           |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,117) | 1:237:C:TRP:HE1  | 1:233:C:LYS:HA  | 7        | 0.2           |
| (1,86)  | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 15       | 0.2           |
| (1,86)  | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 15       | 0.2           |
| (1,86)  | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 15       | 0.2           |
| (1,75)  | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 15       | 0.2           |
| (1,75)  | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 15       | 0.2           |
| (1,75)  | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 15       | 0.2           |
| (1,70)  | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,70)  | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,70)  | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,70)  | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,70)  | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 14       | 0.2           |
| (1,70)  | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 14       | 0.2           |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 14       | 0.2           |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 14       | 0.2           |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 11       | 0.2           |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 14       | 0.2           |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 14       | 0.2           |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 14       | 0.2           |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 14       | 0.2           |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 7        | 0.2           |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 11       | 0.2           |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 7        | 0.2           |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 13       | 0.19          |
| (1,347) | 1:235:C:LEU:H    | 1:232:C:CYS:HA  | 2        | 0.19          |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 3        | 0.19          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 13       | 0.19          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 10       | 0.19          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 2        | 0.19          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 4        | 0.19          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 1        | 0.19          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 10       | 0.19          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 10       | 0.19          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 13       | 0.19          |
| (1,228) | 1:235:C:LEU:H    | 1:232:C:CYS:HA   | 2        | 0.19          |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 3        | 0.19          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA   | 13       | 0.19          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 10       | 0.19          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 2        | 0.19          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 4        | 0.19          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 1        | 0.19          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 10       | 0.19          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 10       | 0.19          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 13       | 0.19          |
| (1,109) | 1:235:C:LEU:H    | 1:232:C:CYS:HA   | 2        | 0.19          |
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 3        | 0.19          |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA   | 13       | 0.19          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 10       | 0.19          |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 2        | 0.19          |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA   | 4        | 0.19          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 1        | 0.19          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 10       | 0.19          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 10       | 0.19          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 11       | 0.18          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 11       | 0.18          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 11       | 0.18          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 11       | 0.18          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 11       | 0.18          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 11       | 0.18          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 11       | 0.18          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 11       | 0.18          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 11       | 0.18          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA   | 10       | 0.18          |
| (1,330) | 1:231:C:VAL:H    | 1:228:C:ALA:HA   | 2        | 0.18          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2  | 1        | 0.18          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3  | 1        | 0.18          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2  | 1        | 0.18          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3  | 1        | 0.18          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2  | 1        | 0.18          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3  | 1        | 0.18          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2  | 2        | 0.18          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3  | 2        | 0.18          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2  | 2        | 0.18          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3  | 2        | 0.18          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2  | 2        | 0.18          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 2        | 0.18          |
| (1,315) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 13       | 0.18          |
| (1,313) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,313) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,313) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 12       | 0.18          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 14       | 0.18          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 10       | 0.18          |
| (1,265) | 1:217:C:TYR:H    | 1:214:C:ILE:HA  | 9        | 0.18          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 13       | 0.18          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 13       | 0.18          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 2        | 0.18          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 10       | 0.18          |
| (1,211) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 2        | 0.18          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 1        | 0.18          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 1        | 0.18          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 1        | 0.18          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 1        | 0.18          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 1        | 0.18          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 1        | 0.18          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 2        | 0.18          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 2        | 0.18          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 2        | 0.18          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 2        | 0.18          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 2        | 0.18          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 2        | 0.18          |
| (1,196) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 13       | 0.18          |
| (1,194) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,194) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,194) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 12       | 0.18          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 14       | 0.18          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 10       | 0.18          |
| (1,146) | 1:217:C:TYR:H    | 1:214:C:ILE:HA  | 9        | 0.18          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 13       | 0.18          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 13       | 0.18          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 2        | 0.18          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 10       | 0.18          |
| (1,92)  | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 2        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 1        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 1        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 1        | 0.18          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 1        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 1        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 1        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 2        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 2        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 2        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 2        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 2        | 0.18          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 2        | 0.18          |
| (1,77)  | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 13       | 0.18          |
| (1,75)  | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,75)  | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,75)  | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 12       | 0.18          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 12       | 0.18          |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 14       | 0.18          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 10       | 0.18          |
| (1,27)  | 1:217:C:TYR:H    | 1:214:C:ILE:HA  | 9        | 0.18          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 13       | 0.18          |
| (1,21)  | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 13       | 0.18          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 2        | 0.18          |
| (1,340) | 1:233:C:LYS:H    | 1:230:C:PHE:HA  | 3        | 0.17          |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 13       | 0.17          |
| (1,335) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,335) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,335) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 12       | 0.17          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 12       | 0.17          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 12       | 0.17          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 11       | 0.17          |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 10       | 0.17          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 9        | 0.17          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 5        | 0.17          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 2        | 0.17          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 6        | 0.17          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 11       | 0.17          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 14       | 0.17          |
| (1,239) | 1:211:C:LEU:H    | 1:210:C:SER:HA  | 2        | 0.17          |
| (1,221) | 1:233:C:LYS:H    | 1:230:C:PHE:HA  | 3        | 0.17          |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 13       | 0.17          |
| (1,216) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,216) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,216) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 12       | 0.17          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 12       | 0.17          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 12       | 0.17          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 11       | 0.17          |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 10       | 0.17          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 9        | 0.17          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 5        | 0.17          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 2        | 0.17          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 6        | 0.17          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 11       | 0.17          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 14       | 0.17          |
| (1,120) | 1:211:C:LEU:H    | 1:210:C:SER:HA  | 2        | 0.17          |
| (1,102) | 1:233:C:LYS:H    | 1:230:C:PHE:HA  | 3        | 0.17          |
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 13       | 0.17          |
| (1,97)  | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,97)  | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,97)  | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 6        | 0.17          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 6        | 0.17          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 6        | 0.17          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 12       | 0.17          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 12       | 0.17          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 12       | 0.17          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 12       | 0.17          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 11       | 0.17          |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 10       | 0.17          |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 9        | 0.17          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 5        | 0.17          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 2        | 0.17          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 6        | 0.17          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 11       | 0.17          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 14       | 0.17          |
| (1,1)   | 1:211:C:LEU:H    | 1:210:C:SER:HA  | 2        | 0.17          |
| (1,352) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 2        | 0.16          |
| (1,335) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 11       | 0.16          |
| (1,335) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 11       | 0.16          |
| (1,335) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 11       | 0.16          |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 7        | 0.16          |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 7        | 0.16          |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 7        | 0.16          |
| (1,313) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 13       | 0.16          |
| (1,313) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 13       | 0.16          |
| (1,313) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 13       | 0.16          |
| (1,309) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 8        | 0.16          |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 15       | 0.16          |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 15       | 0.16          |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 15       | 0.16          |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 15       | 0.16          |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 15       | 0.16          |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 15       | 0.16          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 3        | 0.16          |
| (1,302) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 4        | 0.16          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 1        | 0.16          |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 2        | 0.16          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 1        | 0.16          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 5        | 0.16          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 7        | 0.16          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 9        | 0.16          |
| (1,252) | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA  | 3        | 0.16          |
| (1,252) | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA  | 3        | 0.16          |
| (1,252) | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA  | 3        | 0.16          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 9        | 0.16          |
| (1,249) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 11       | 0.16          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 1        | 0.16          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 13       | 0.16          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 15       | 0.16          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 2        | 0.16          |
| (1,233) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 2        | 0.16          |
| (1,216) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 11       | 0.16          |
| (1,216) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 11       | 0.16          |
| (1,216) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 11       | 0.16          |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 7        | 0.16          |
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 7        | 0.16          |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 7        | 0.16          |
| (1,194) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 13       | 0.16          |
| (1,194) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 13       | 0.16          |
| (1,194) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 13       | 0.16          |
| (1,190) | 1:227:C:VAL:H    | 1:224:C:VAL:HA  | 8        | 0.16          |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 15       | 0.16          |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 15       | 0.16          |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 15       | 0.16          |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 15       | 0.16          |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 15       | 0.16          |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 15       | 0.16          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 3        | 0.16          |
| (1,183) | 1:225:C:LEU:H    | 1:222:C:ALA:HA  | 4        | 0.16          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 1        | 0.16          |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 2        | 0.16          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 1        | 0.16          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 5        | 0.16          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 7        | 0.16          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 9        | 0.16          |
| (1,133) | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA  | 3        | 0.16          |
| (1,133) | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA  | 3        | 0.16          |
| (1,133) | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA  | 3        | 0.16          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 9        | 0.16          |
| (1,130) | 1:214:C:ILE:H    | 1:211:C:LEU:HA  | 11       | 0.16          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 1        | 0.16          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 13       | 0.16          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 15       | 0.16          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 2        | 0.16          |
| (1,114) | 1:237:C:TRP:H    | 1:233:C:LYS:HA  | 2        | 0.16          |
| (1,97)  | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 11       | 0.16          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,97)  | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA   | 11       | 0.16          |
| (1,97)  | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA   | 11       | 0.16          |
| (1,86)  | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 7        | 0.16          |
| (1,86)  | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 7        | 0.16          |
| (1,86)  | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 7        | 0.16          |
| (1,75)  | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA   | 13       | 0.16          |
| (1,75)  | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA   | 13       | 0.16          |
| (1,75)  | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA   | 13       | 0.16          |
| (1,71)  | 1:227:C:VAL:H    | 1:224:C:VAL:HA   | 8        | 0.16          |
| (1,70)  | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1  | 15       | 0.16          |
| (1,70)  | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2  | 15       | 0.16          |
| (1,70)  | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1  | 15       | 0.16          |
| (1,70)  | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2  | 15       | 0.16          |
| (1,70)  | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1  | 15       | 0.16          |
| (1,70)  | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2  | 15       | 0.16          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 3        | 0.16          |
| (1,64)  | 1:225:C:LEU:H    | 1:222:C:ALA:HA   | 4        | 0.16          |
| (1,60)  | 1:224:C:VAL:H    | 1:221:C:ALA:HA   | 1        | 0.16          |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA   | 2        | 0.16          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 1        | 0.16          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 5        | 0.16          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 7        | 0.16          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 9        | 0.16          |
| (1,14)  | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA   | 3        | 0.16          |
| (1,14)  | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA   | 3        | 0.16          |
| (1,14)  | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA   | 3        | 0.16          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 9        | 0.16          |
| (1,11)  | 1:214:C:ILE:H    | 1:211:C:LEU:HA   | 11       | 0.16          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 1        | 0.16          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 13       | 0.16          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 15       | 0.16          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA   | 2        | 0.16          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 11       | 0.15          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 11       | 0.15          |
| (1,363) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 11       | 0.15          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 11       | 0.15          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 11       | 0.15          |
| (1,362) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 11       | 0.15          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG21 | 11       | 0.15          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG22 | 11       | 0.15          |
| (1,361) | 1:220:C:VAL:H    | 1:218:C:VAL:HG23 | 11       | 0.15          |
| (1,357) | 1:239:C:LYS:H    | 1:238:C:LYS:H    | 13       | 0.15          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,356) | 1:238:C:LYS:H    | 1:239:C:LYS:H   | 13       | 0.15          |
| (1,343) | 1:234:C:SER:H    | 1:231:C:VAL:HA  | 15       | 0.15          |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 5        | 0.15          |
| (1,335) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 3        | 0.15          |
| (1,335) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 3        | 0.15          |
| (1,335) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 3        | 0.15          |
| (1,331) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 11       | 0.15          |
| (1,330) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 5        | 0.15          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 8        | 0.15          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 8        | 0.15          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 8        | 0.15          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 8        | 0.15          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 8        | 0.15          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 8        | 0.15          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 11       | 0.15          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 11       | 0.15          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 11       | 0.15          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 11       | 0.15          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 11       | 0.15          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 11       | 0.15          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 1        | 0.15          |
| (1,313) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 5        | 0.15          |
| (1,313) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 5        | 0.15          |
| (1,313) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 5        | 0.15          |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 12       | 0.15          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 1        | 0.15          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 3        | 0.15          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 4        | 0.15          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 10       | 0.15          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 12       | 0.15          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 14       | 0.15          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 15       | 0.15          |
| (1,254) | 1:214:C:ILE:HG21 | 1:218:C:VAL:H   | 13       | 0.15          |
| (1,254) | 1:214:C:ILE:HG22 | 1:218:C:VAL:H   | 13       | 0.15          |
| (1,254) | 1:214:C:ILE:HG23 | 1:218:C:VAL:H   | 13       | 0.15          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 2        | 0.15          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 8        | 0.15          |
| (1,241) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 6        | 0.15          |
| (1,241) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 6        | 0.15          |
| (1,241) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 6        | 0.15          |
| (1,238) | 1:239:C:LYS:H    | 1:238:C:LYS:H   | 13       | 0.15          |
| (1,237) | 1:238:C:LYS:H    | 1:239:C:LYS:H   | 13       | 0.15          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,224) | 1:234:C:SER:H    | 1:231:C:VAL:HA  | 15       | 0.15          |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 5        | 0.15          |
| (1,216) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 3        | 0.15          |
| (1,216) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 3        | 0.15          |
| (1,216) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 3        | 0.15          |
| (1,212) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 11       | 0.15          |
| (1,211) | 1:231:C:VAL:H    | 1:228:C:ALA:HA  | 5        | 0.15          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 8        | 0.15          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 8        | 0.15          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 8        | 0.15          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 8        | 0.15          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 8        | 0.15          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 8        | 0.15          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 11       | 0.15          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 11       | 0.15          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 11       | 0.15          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 11       | 0.15          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 11       | 0.15          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 11       | 0.15          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 1        | 0.15          |
| (1,194) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 5        | 0.15          |
| (1,194) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 5        | 0.15          |
| (1,194) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 5        | 0.15          |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 12       | 0.15          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 1        | 0.15          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 3        | 0.15          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 4        | 0.15          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 10       | 0.15          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 12       | 0.15          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 14       | 0.15          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 15       | 0.15          |
| (1,135) | 1:214:C:ILE:HG21 | 1:218:C:VAL:H   | 13       | 0.15          |
| (1,135) | 1:214:C:ILE:HG22 | 1:218:C:VAL:H   | 13       | 0.15          |
| (1,135) | 1:214:C:ILE:HG23 | 1:218:C:VAL:H   | 13       | 0.15          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 2        | 0.15          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 8        | 0.15          |
| (1,122) | 1:211:C:LEU:HD21 | 1:215:C:ILE:H   | 6        | 0.15          |
| (1,122) | 1:211:C:LEU:HD22 | 1:215:C:ILE:H   | 6        | 0.15          |
| (1,122) | 1:211:C:LEU:HD23 | 1:215:C:ILE:H   | 6        | 0.15          |
| (1,119) | 1:239:C:LYS:H    | 1:238:C:LYS:H   | 13       | 0.15          |
| (1,118) | 1:238:C:LYS:H    | 1:239:C:LYS:H   | 13       | 0.15          |
| (1,105) | 1:234:C:SER:H    | 1:231:C:VAL:HA  | 15       | 0.15          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 5        | 0.15          |
| (1,97)  | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA   | 3        | 0.15          |
| (1,97)  | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA   | 3        | 0.15          |
| (1,97)  | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA   | 3        | 0.15          |
| (1,93)  | 1:231:C:VAL:H    | 1:230:C:PHE:HA   | 11       | 0.15          |
| (1,92)  | 1:231:C:VAL:H    | 1:228:C:ALA:HA   | 5        | 0.15          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2  | 8        | 0.15          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3  | 8        | 0.15          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2  | 8        | 0.15          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3  | 8        | 0.15          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2  | 8        | 0.15          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3  | 8        | 0.15          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2  | 11       | 0.15          |
| (1,87)  | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3  | 11       | 0.15          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2  | 11       | 0.15          |
| (1,87)  | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3  | 11       | 0.15          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2  | 11       | 0.15          |
| (1,87)  | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3  | 11       | 0.15          |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA   | 1        | 0.15          |
| (1,75)  | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA   | 5        | 0.15          |
| (1,75)  | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA   | 5        | 0.15          |
| (1,75)  | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA   | 5        | 0.15          |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA   | 12       | 0.15          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 1        | 0.15          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 3        | 0.15          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 4        | 0.15          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 10       | 0.15          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 12       | 0.15          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 14       | 0.15          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 15       | 0.15          |
| (1,16)  | 1:214:C:ILE:HG21 | 1:218:C:VAL:H    | 13       | 0.15          |
| (1,16)  | 1:214:C:ILE:HG22 | 1:218:C:VAL:H    | 13       | 0.15          |
| (1,16)  | 1:214:C:ILE:HG23 | 1:218:C:VAL:H    | 13       | 0.15          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 2        | 0.15          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 8        | 0.15          |
| (1,3)   | 1:211:C:LEU:HD21 | 1:215:C:ILE:H    | 6        | 0.15          |
| (1,3)   | 1:211:C:LEU:HD22 | 1:215:C:ILE:H    | 6        | 0.15          |
| (1,3)   | 1:211:C:LEU:HD23 | 1:215:C:ILE:H    | 6        | 0.15          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 1        | 0.14          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 1        | 0.14          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 1        | 0.14          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 1        | 0.14          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 1        | 0.14          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 1        | 0.14          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 1        | 0.14          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 1        | 0.14          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 1        | 0.14          |
| (1,331) | 1:231:C:VAL:H    | 1:230:C:PHE:HA   | 6        | 0.14          |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,306) | 1:226:C:ILE:H    | 1:225:C:LEU:HA   | 6        | 0.14          |
| (1,306) | 1:226:C:ILE:H    | 1:225:C:LEU:HA   | 14       | 0.14          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 5        | 0.14          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 9        | 0.14          |
| (1,271) | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 8        | 0.14          |
| (1,252) | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA   | 14       | 0.14          |
| (1,252) | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA   | 14       | 0.14          |
| (1,252) | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA   | 14       | 0.14          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 4        | 0.14          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 6        | 0.14          |
| (1,243) | 1:212:C:SER:H    | 1:211:C:LEU:H    | 5        | 0.14          |
| (1,212) | 1:231:C:VAL:H    | 1:230:C:PHE:HA   | 6        | 0.14          |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,187) | 1:226:C:ILE:H    | 1:225:C:LEU:HA   | 6        | 0.14          |
| (1,187) | 1:226:C:ILE:H    | 1:225:C:LEU:HA   | 14       | 0.14          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 5        | 0.14          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 9        | 0.14          |
| (1,152) | 1:218:C:VAL:H    | 1:217:C:TYR:HA   | 8        | 0.14          |
| (1,133) | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA   | 14       | 0.14          |
| (1,133) | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA   | 14       | 0.14          |
| (1,133) | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA   | 14       | 0.14          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 4        | 0.14          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 6        | 0.14          |
| (1,124) | 1:212:C:SER:H    | 1:211:C:LEU:H    | 5        | 0.14          |
| (1,93)  | 1:231:C:VAL:H    | 1:230:C:PHE:HA   | 6        | 0.14          |
| (1,86)  | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,86)  | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,86)  | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 5        | 0.14          |
| (1,68)  | 1:226:C:ILE:H    | 1:225:C:LEU:HA   | 6        | 0.14          |
| (1,68)  | 1:226:C:ILE:H    | 1:225:C:LEU:HA   | 14       | 0.14          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA   | 5        | 0.14          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 9        | 0.14          |
| (1,33)  | 1:218:C:VAL:H    | 1:217:C:TYR:HA  | 8        | 0.14          |
| (1,14)  | 1:214:C:ILE:HG21 | 1:211:C:LEU:HA  | 14       | 0.14          |
| (1,14)  | 1:214:C:ILE:HG22 | 1:211:C:LEU:HA  | 14       | 0.14          |
| (1,14)  | 1:214:C:ILE:HG23 | 1:211:C:LEU:HA  | 14       | 0.14          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 4        | 0.14          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 6        | 0.14          |
| (1,5)   | 1:212:C:SER:H    | 1:211:C:LEU:H   | 5        | 0.14          |
| (1,353) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 5        | 0.13          |
| (1,331) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 3        | 0.13          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 2        | 0.13          |
| (1,315) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 12       | 0.13          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 8        | 0.13          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 8        | 0.13          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 8        | 0.13          |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 5        | 0.13          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 11       | 0.13          |
| (1,279) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 4        | 0.13          |
| (1,279) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 8        | 0.13          |
| (1,279) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 12       | 0.13          |
| (1,279) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 14       | 0.13          |
| (1,279) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 15       | 0.13          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 2        | 0.13          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 2        | 0.13          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 2        | 0.13          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 2        | 0.13          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 2        | 0.13          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 2        | 0.13          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 13       | 0.13          |
| (1,262) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 13       | 0.13          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 13       | 0.13          |
| (1,262) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 13       | 0.13          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 13       | 0.13          |
| (1,262) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 13       | 0.13          |
| (1,256) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 7        | 0.13          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 12       | 0.13          |
| (1,246) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 14       | 0.13          |
| (1,234) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 5        | 0.13          |
| (1,212) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 3        | 0.13          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 2        | 0.13          |
| (1,196) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 12       | 0.13          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 8        | 0.13          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 8        | 0.13          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 8        | 0.13          |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 5        | 0.13          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 11       | 0.13          |
| (1,160) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 4        | 0.13          |
| (1,160) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 8        | 0.13          |
| (1,160) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 12       | 0.13          |
| (1,160) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 14       | 0.13          |
| (1,160) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 15       | 0.13          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 2        | 0.13          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 2        | 0.13          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 2        | 0.13          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 2        | 0.13          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 2        | 0.13          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 2        | 0.13          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 13       | 0.13          |
| (1,143) | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 13       | 0.13          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 13       | 0.13          |
| (1,143) | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 13       | 0.13          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2 | 13       | 0.13          |
| (1,143) | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3 | 13       | 0.13          |
| (1,137) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 7        | 0.13          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 12       | 0.13          |
| (1,127) | 1:213:C:GLY:H    | 1:212:C:SER:HA  | 14       | 0.13          |
| (1,115) | 1:237:C:TRP:H    | 1:234:C:SER:HA  | 5        | 0.13          |
| (1,93)  | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 3        | 0.13          |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 2        | 0.13          |
| (1,77)  | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 12       | 0.13          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 8        | 0.13          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 8        | 0.13          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 8        | 0.13          |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 5        | 0.13          |
| (1,46)  | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 11       | 0.13          |
| (1,41)  | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 4        | 0.13          |
| (1,41)  | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 8        | 0.13          |
| (1,41)  | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 12       | 0.13          |
| (1,41)  | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 14       | 0.13          |
| (1,41)  | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 15       | 0.13          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2 | 2        | 0.13          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3 | 2        | 0.13          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2 | 2        | 0.13          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3 | 2        | 0.13          |

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| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2  | 2        | 0.13          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3  | 2        | 0.13          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB2  | 13       | 0.13          |
| (1,24)  | 1:216:C:ILE:HD11 | 1:212:C:SER:HB3  | 13       | 0.13          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB2  | 13       | 0.13          |
| (1,24)  | 1:216:C:ILE:HD12 | 1:212:C:SER:HB3  | 13       | 0.13          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB2  | 13       | 0.13          |
| (1,24)  | 1:216:C:ILE:HD13 | 1:212:C:SER:HB3  | 13       | 0.13          |
| (1,18)  | 1:215:C:ILE:H    | 1:214:C:ILE:HA   | 7        | 0.13          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 12       | 0.13          |
| (1,8)   | 1:213:C:GLY:H    | 1:212:C:SER:HA   | 14       | 0.13          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 4        | 0.12          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 4        | 0.12          |
| (1,366) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 4        | 0.12          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 4        | 0.12          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 4        | 0.12          |
| (1,365) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 4        | 0.12          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG21 | 4        | 0.12          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG22 | 4        | 0.12          |
| (1,364) | 1:222:C:ALA:H    | 1:223:C:VAL:HG23 | 4        | 0.12          |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA   | 10       | 0.12          |
| (1,335) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA   | 4        | 0.12          |
| (1,335) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA   | 4        | 0.12          |
| (1,335) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA   | 4        | 0.12          |
| (1,331) | 1:231:C:VAL:H    | 1:230:C:PHE:HA   | 5        | 0.12          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2  | 14       | 0.12          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3  | 14       | 0.12          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2  | 14       | 0.12          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3  | 14       | 0.12          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2  | 14       | 0.12          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3  | 14       | 0.12          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2  | 15       | 0.12          |
| (1,325) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3  | 15       | 0.12          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2  | 15       | 0.12          |
| (1,325) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3  | 15       | 0.12          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2  | 15       | 0.12          |
| (1,325) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3  | 15       | 0.12          |
| (1,324) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA   | 11       | 0.12          |
| (1,324) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA   | 11       | 0.12          |
| (1,324) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA   | 11       | 0.12          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA   | 5        | 0.12          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA   | 14       | 0.12          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 15       | 0.12          |
| (1,315) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 1        | 0.12          |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,308) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,308) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,308) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,298) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 4        | 0.12          |
| (1,294) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 8        | 0.12          |
| (1,294) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 13       | 0.12          |
| (1,284) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 7        | 0.12          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 12       | 0.12          |
| (1,279) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 3        | 0.12          |
| (1,279) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 9        | 0.12          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 1        | 0.12          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 14       | 0.12          |
| (1,259) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 14       | 0.12          |
| (1,256) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 9        | 0.12          |
| (1,256) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 10       | 0.12          |
| (1,256) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 11       | 0.12          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 3        | 0.12          |
| (1,253) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,253) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 3        | 0.12          |
| (1,253) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,253) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 3        | 0.12          |
| (1,253) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,253) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 3        | 0.12          |
| (1,239) | 1:211:C:LEU:H    | 1:210:C:SER:HA  | 15       | 0.12          |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 10       | 0.12          |
| (1,216) | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 4        | 0.12          |
| (1,216) | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 4        | 0.12          |
| (1,216) | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 4        | 0.12          |
| (1,212) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 5        | 0.12          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 14       | 0.12          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 14       | 0.12          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 14       | 0.12          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 14       | 0.12          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 14       | 0.12          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 14       | 0.12          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 15       | 0.12          |
| (1,206) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 15       | 0.12          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 15       | 0.12          |
| (1,206) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 15       | 0.12          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 15       | 0.12          |
| (1,206) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 15       | 0.12          |
| (1,205) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 11       | 0.12          |
| (1,205) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 11       | 0.12          |
| (1,205) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 11       | 0.12          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 5        | 0.12          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 14       | 0.12          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 15       | 0.12          |
| (1,196) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 1        | 0.12          |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,189) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,189) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,189) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,179) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 4        | 0.12          |
| (1,175) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 8        | 0.12          |
| (1,175) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 13       | 0.12          |
| (1,165) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 7        | 0.12          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 12       | 0.12          |
| (1,160) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 3        | 0.12          |
| (1,160) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 9        | 0.12          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 1        | 0.12          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 14       | 0.12          |
| (1,140) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 14       | 0.12          |
| (1,137) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 9        | 0.12          |
| (1,137) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 10       | 0.12          |
| (1,137) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 11       | 0.12          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 3        | 0.12          |
| (1,134) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,134) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 3        | 0.12          |
| (1,134) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,134) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 3        | 0.12          |
| (1,134) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,134) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 3        | 0.12          |
| (1,120) | 1:211:C:LEU:H    | 1:210:C:SER:HA  | 15       | 0.12          |
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 10       | 0.12          |
| (1,97)  | 1:231:C:VAL:HG21 | 1:228:C:ALA:HA  | 4        | 0.12          |
| (1,97)  | 1:231:C:VAL:HG22 | 1:228:C:ALA:HA  | 4        | 0.12          |
| (1,97)  | 1:231:C:VAL:HG23 | 1:228:C:ALA:HA  | 4        | 0.12          |

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| Key    | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|--------|------------------|-----------------|----------|---------------|
| (1,93) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 5        | 0.12          |
| (1,87) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 14       | 0.12          |
| (1,87) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 14       | 0.12          |
| (1,87) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 14       | 0.12          |
| (1,87) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 14       | 0.12          |
| (1,87) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 14       | 0.12          |
| (1,87) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 14       | 0.12          |
| (1,87) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB2 | 15       | 0.12          |
| (1,87) | 1:229:C:VAL:HG21 | 1:233:C:LYS:HB3 | 15       | 0.12          |
| (1,87) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB2 | 15       | 0.12          |
| (1,87) | 1:229:C:VAL:HG22 | 1:233:C:LYS:HB3 | 15       | 0.12          |
| (1,87) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB2 | 15       | 0.12          |
| (1,87) | 1:229:C:VAL:HG23 | 1:233:C:LYS:HB3 | 15       | 0.12          |
| (1,86) | 1:229:C:VAL:HG11 | 1:225:C:LEU:HA  | 11       | 0.12          |
| (1,86) | 1:229:C:VAL:HG12 | 1:225:C:LEU:HA  | 11       | 0.12          |
| (1,86) | 1:229:C:VAL:HG13 | 1:225:C:LEU:HA  | 11       | 0.12          |
| (1,82) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 5        | 0.12          |
| (1,82) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 14       | 0.12          |
| (1,82) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 15       | 0.12          |
| (1,77) | 1:228:C:ALA:H    | 1:224:C:VAL:HA  | 1        | 0.12          |
| (1,70) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,70) | 1:226:C:ILE:HG21 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,70) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,70) | 1:226:C:ILE:HG22 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,70) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE1 | 6        | 0.12          |
| (1,70) | 1:226:C:ILE:HG23 | 1:230:C:PHE:HE2 | 6        | 0.12          |
| (1,60) | 1:224:C:VAL:H    | 1:221:C:ALA:HA  | 4        | 0.12          |
| (1,56) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 8        | 0.12          |
| (1,56) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 13       | 0.12          |
| (1,46) | 1:221:C:ALA:H    | 1:218:C:VAL:HA  | 7        | 0.12          |
| (1,45) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 12       | 0.12          |
| (1,41) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 3        | 0.12          |
| (1,41) | 1:220:C:VAL:H    | 1:219:C:THR:HA  | 9        | 0.12          |
| (1,40) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 1        | 0.12          |
| (1,21) | 1:216:C:ILE:H    | 1:213:C:GLY:HA2 | 14       | 0.12          |
| (1,21) | 1:216:C:ILE:H    | 1:213:C:GLY:HA3 | 14       | 0.12          |
| (1,18) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 9        | 0.12          |
| (1,18) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 10       | 0.12          |
| (1,18) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 11       | 0.12          |
| (1,17) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 3        | 0.12          |
| (1,15) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,15) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 3        | 0.12          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,15)  | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,15)  | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 3        | 0.12          |
| (1,15)  | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 3        | 0.12          |
| (1,15)  | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 3        | 0.12          |
| (1,1)   | 1:211:C:LEU:H    | 1:210:C:SER:HA  | 15       | 0.12          |
| (1,340) | 1:233:C:LYS:H    | 1:230:C:PHE:HA  | 4        | 0.11          |
| (1,331) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 2        | 0.11          |
| (1,331) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 4        | 0.11          |
| (1,331) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 7        | 0.11          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 6        | 0.11          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 8        | 0.11          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 10       | 0.11          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 11       | 0.11          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 12       | 0.11          |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 13       | 0.11          |
| (1,316) | 1:228:C:ALA:H    | 1:227:C:VAL:HA  | 4        | 0.11          |
| (1,306) | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 9        | 0.11          |
| (1,301) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,301) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,301) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,294) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 12       | 0.11          |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 4        | 0.11          |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 9        | 0.11          |
| (1,283) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 15       | 0.11          |
| (1,278) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 6        | 0.11          |
| (1,255) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 14       | 0.11          |
| (1,253) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,253) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 11       | 0.11          |
| (1,253) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,253) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 11       | 0.11          |
| (1,253) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,253) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 11       | 0.11          |
| (1,242) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 11       | 0.11          |
| (1,221) | 1:233:C:LYS:H    | 1:230:C:PHE:HA  | 4        | 0.11          |
| (1,212) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 2        | 0.11          |
| (1,212) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 4        | 0.11          |
| (1,212) | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 7        | 0.11          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 6        | 0.11          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 8        | 0.11          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 10       | 0.11          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 11       | 0.11          |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 12       | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 13       | 0.11          |
| (1,197) | 1:228:C:ALA:H    | 1:227:C:VAL:HA  | 4        | 0.11          |
| (1,187) | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 9        | 0.11          |
| (1,182) | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,182) | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,182) | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,175) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 12       | 0.11          |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 4        | 0.11          |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 9        | 0.11          |
| (1,164) | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 15       | 0.11          |
| (1,159) | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 6        | 0.11          |
| (1,136) | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 14       | 0.11          |
| (1,134) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,134) | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 11       | 0.11          |
| (1,134) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,134) | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 11       | 0.11          |
| (1,134) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,134) | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 11       | 0.11          |
| (1,123) | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 11       | 0.11          |
| (1,102) | 1:233:C:LYS:H    | 1:230:C:PHE:HA  | 4        | 0.11          |
| (1,93)  | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 2        | 0.11          |
| (1,93)  | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 4        | 0.11          |
| (1,93)  | 1:231:C:VAL:H    | 1:230:C:PHE:HA  | 7        | 0.11          |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 6        | 0.11          |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 8        | 0.11          |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 10       | 0.11          |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 11       | 0.11          |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 12       | 0.11          |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 13       | 0.11          |
| (1,78)  | 1:228:C:ALA:H    | 1:227:C:VAL:HA  | 4        | 0.11          |
| (1,68)  | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 9        | 0.11          |
| (1,63)  | 1:224:C:VAL:HG11 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,63)  | 1:224:C:VAL:HG12 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,63)  | 1:224:C:VAL:HG13 | 1:221:C:ALA:HA  | 2        | 0.11          |
| (1,56)  | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 12       | 0.11          |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 4        | 0.11          |
| (1,55)  | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 9        | 0.11          |
| (1,45)  | 1:221:C:ALA:H    | 1:217:C:TYR:HA  | 15       | 0.11          |
| (1,40)  | 1:220:C:VAL:H    | 1:217:C:TYR:HA  | 6        | 0.11          |
| (1,17)  | 1:215:C:ILE:H    | 1:212:C:SER:HA  | 14       | 0.11          |
| (1,15)  | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,15)  | 1:214:C:ILE:HD11 | 1:217:C:TYR:HD2 | 11       | 0.11          |

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| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,15)  | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,15)  | 1:214:C:ILE:HD12 | 1:217:C:TYR:HD2 | 11       | 0.11          |
| (1,15)  | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD1 | 11       | 0.11          |
| (1,15)  | 1:214:C:ILE:HD13 | 1:217:C:TYR:HD2 | 11       | 0.11          |
| (1,4)   | 1:212:C:SER:H    | 1:211:C:LEU:HA  | 11       | 0.11          |
| (1,344) | 1:234:C:SER:H    | 1:233:C:LYS:HA  | 5        | 0.1           |
| (1,336) | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 8        | 0.1           |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 4        | 0.1           |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 7        | 0.1           |
| (1,320) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 9        | 0.1           |
| (1,316) | 1:228:C:ALA:H    | 1:227:C:VAL:HA  | 2        | 0.1           |
| (1,316) | 1:228:C:ALA:H    | 1:227:C:VAL:HA  | 5        | 0.1           |
| (1,313) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 1        | 0.1           |
| (1,313) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 1        | 0.1           |
| (1,313) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 1        | 0.1           |
| (1,306) | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 1        | 0.1           |
| (1,306) | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 3        | 0.1           |
| (1,294) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 14       | 0.1           |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 3        | 0.1           |
| (1,293) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 7        | 0.1           |
| (1,256) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 15       | 0.1           |
| (1,225) | 1:234:C:SER:H    | 1:233:C:LYS:HA  | 5        | 0.1           |
| (1,217) | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 8        | 0.1           |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 4        | 0.1           |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 7        | 0.1           |
| (1,201) | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 9        | 0.1           |
| (1,197) | 1:228:C:ALA:H    | 1:227:C:VAL:HA  | 2        | 0.1           |
| (1,197) | 1:228:C:ALA:H    | 1:227:C:VAL:HA  | 5        | 0.1           |
| (1,194) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA  | 1        | 0.1           |
| (1,194) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA  | 1        | 0.1           |
| (1,194) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA  | 1        | 0.1           |
| (1,187) | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 1        | 0.1           |
| (1,187) | 1:226:C:ILE:H    | 1:225:C:LEU:HA  | 3        | 0.1           |
| (1,175) | 1:223:C:VAL:H    | 1:222:C:ALA:HA  | 14       | 0.1           |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 3        | 0.1           |
| (1,174) | 1:223:C:VAL:H    | 1:220:C:VAL:HA  | 7        | 0.1           |
| (1,137) | 1:215:C:ILE:H    | 1:214:C:ILE:HA  | 15       | 0.1           |
| (1,106) | 1:234:C:SER:H    | 1:233:C:LYS:HA  | 5        | 0.1           |
| (1,98)  | 1:232:C:CYS:H    | 1:229:C:VAL:HA  | 8        | 0.1           |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 4        | 0.1           |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 7        | 0.1           |
| (1,82)  | 1:229:C:VAL:H    | 1:228:C:ALA:HA  | 9        | 0.1           |

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| Key    | Atom-1           | Atom-2         | Model ID | Violation (Å) |
|--------|------------------|----------------|----------|---------------|
| (1,78) | 1:228:C:ALA:H    | 1:227:C:VAL:HA | 2        | 0.1           |
| (1,78) | 1:228:C:ALA:H    | 1:227:C:VAL:HA | 5        | 0.1           |
| (1,75) | 1:227:C:VAL:HG11 | 1:224:C:VAL:HA | 1        | 0.1           |
| (1,75) | 1:227:C:VAL:HG12 | 1:224:C:VAL:HA | 1        | 0.1           |
| (1,75) | 1:227:C:VAL:HG13 | 1:224:C:VAL:HA | 1        | 0.1           |
| (1,68) | 1:226:C:ILE:H    | 1:225:C:LEU:HA | 1        | 0.1           |
| (1,68) | 1:226:C:ILE:H    | 1:225:C:LEU:HA | 3        | 0.1           |
| (1,56) | 1:223:C:VAL:H    | 1:222:C:ALA:HA | 14       | 0.1           |
| (1,55) | 1:223:C:VAL:H    | 1:220:C:VAL:HA | 3        | 0.1           |
| (1,55) | 1:223:C:VAL:H    | 1:220:C:VAL:HA | 7        | 0.1           |
| (1,18) | 1:215:C:ILE:H    | 1:214:C:ILE:HA | 15       | 0.1           |

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

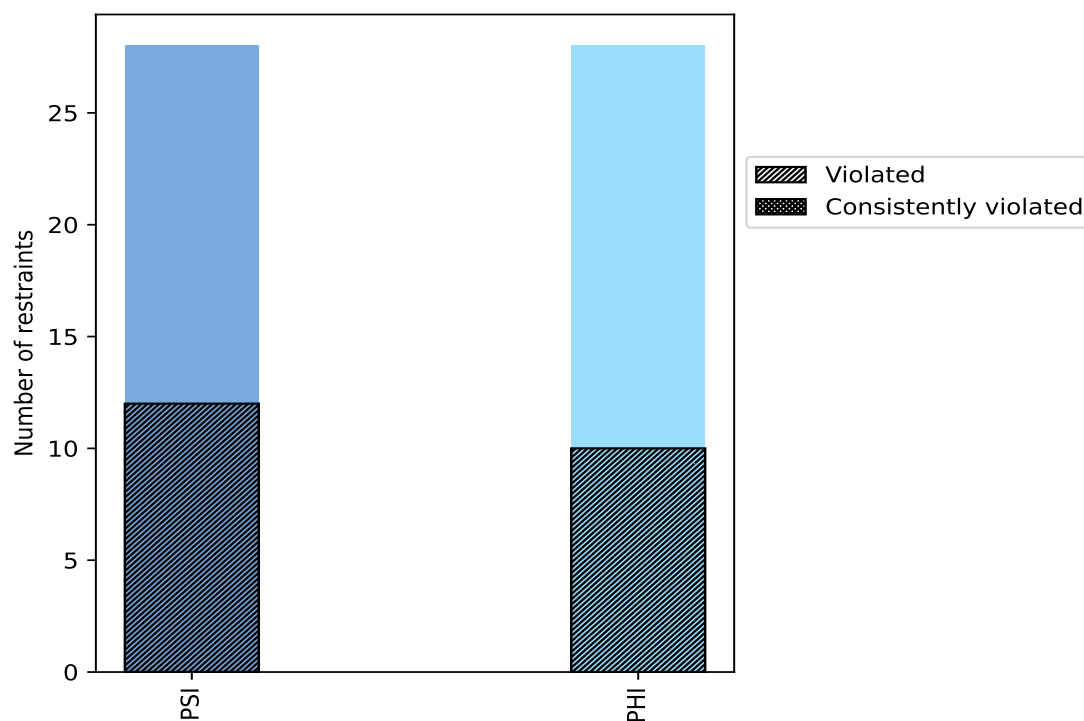
### 10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 28    | 50.0           | 12                    | 42.9           | 21.4           | 0                                  | 0.0            | 0.0            |
| PHI        | 28    | 50.0           | 10                    | 35.7           | 17.9           | 0                                  | 0.0            | 0.0            |
| Total      | 56    | 100.0          | 22                    | 39.3           | 39.3           | 0                                  | 0.0            | 0.0            |

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

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



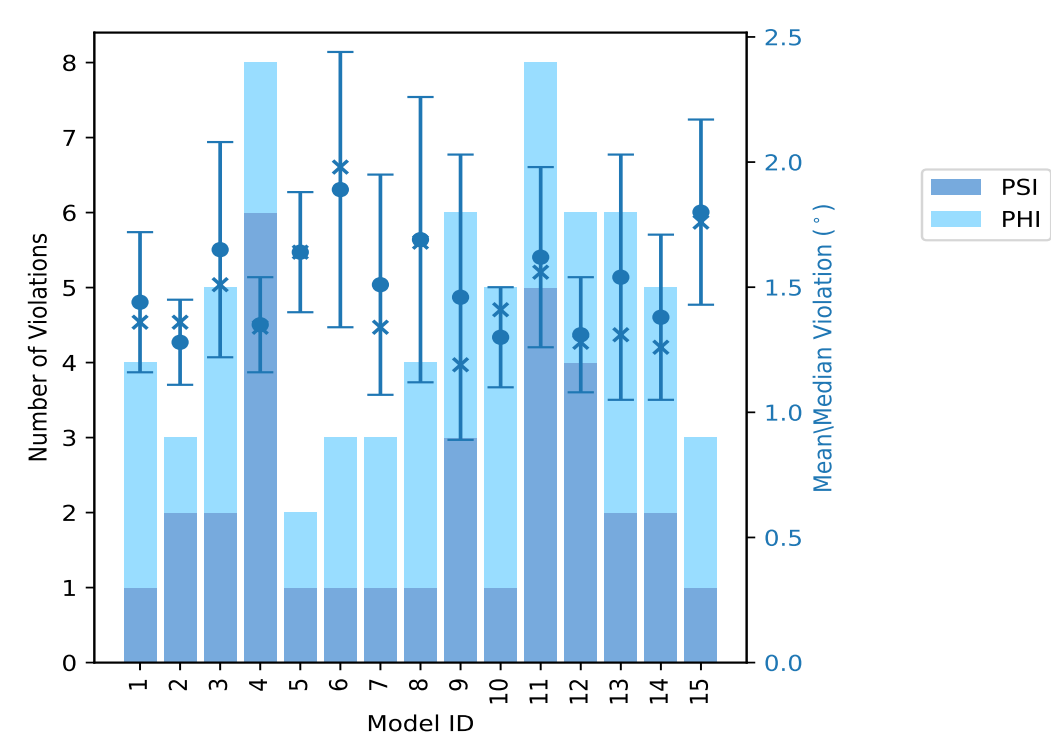
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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        | 1                    | 3   | 4     | 1.44     | 1.89    | 0.28   | 1.36       |
| 2        | 2                    | 1   | 3     | 1.28     | 1.43    | 0.17   | 1.36       |
| 3        | 2                    | 3   | 5     | 1.65     | 2.35    | 0.43   | 1.51       |
| 4        | 6                    | 2   | 8     | 1.35     | 1.68    | 0.19   | 1.34       |
| 5        | 1                    | 1   | 2     | 1.64     | 1.88    | 0.24   | 1.64       |
| 6        | 1                    | 2   | 3     | 1.89     | 2.52    | 0.55   | 1.98       |
| 7        | 1                    | 2   | 3     | 1.51     | 2.11    | 0.44   | 1.34       |
| 8        | 1                    | 3   | 4     | 1.69     | 2.36    | 0.57   | 1.68       |
| 9        | 3                    | 3   | 6     | 1.46     | 2.67    | 0.57   | 1.19       |
| 10       | 1                    | 4   | 5     | 1.3      | 1.56    | 0.2    | 1.41       |
| 11       | 5                    | 3   | 8     | 1.62     | 2.15    | 0.36   | 1.56       |
| 12       | 4                    | 2   | 6     | 1.31     | 1.61    | 0.23   | 1.28       |
| 13       | 2                    | 4   | 6     | 1.54     | 2.39    | 0.49   | 1.31       |
| 14       | 2                    | 3   | 5     | 1.38     | 1.95    | 0.33   | 1.26       |
| 15       | 1                    | 2   | 3     | 1.8      | 2.27    | 0.37   | 1.76       |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

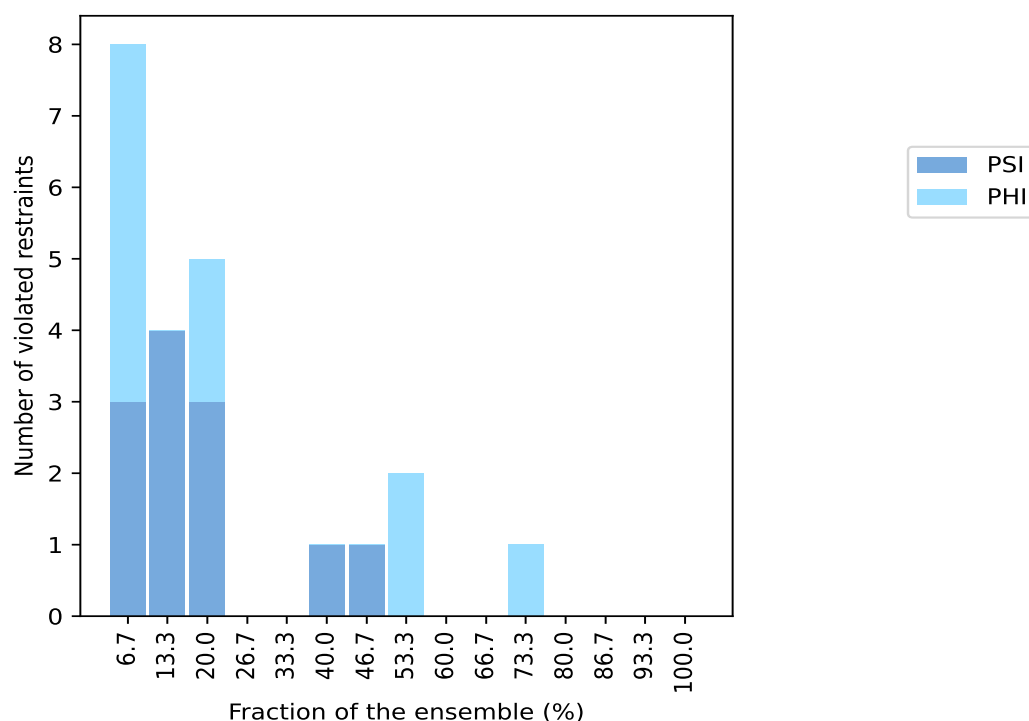
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 3                             | 5   | 8     | 1                        | 6.7   |
| 4                             | 0   | 4     | 2                        | 13.3  |
| 3                             | 2   | 5     | 3                        | 20.0  |
| 0                             | 0   | 0     | 4                        | 26.7  |
| 0                             | 0   | 0     | 5                        | 33.3  |
| 1                             | 0   | 1     | 6                        | 40.0  |
| 1                             | 0   | 1     | 7                        | 46.7  |
| 0                             | 2   | 2     | 8                        | 53.3  |
| 0                             | 0   | 0     | 9                        | 60.0  |
| 0                             | 0   | 0     | 10                       | 66.7  |
| 0                             | 1   | 1     | 11                       | 73.3  |
| 0                             | 0   | 0     | 12                       | 80.0  |
| 0                             | 0   | 0     | 13                       | 86.7  |
| 0                             | 0   | 0     | 14                       | 93.3  |
| 0                             | 0   | 0     | 15                       | 100.0 |

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

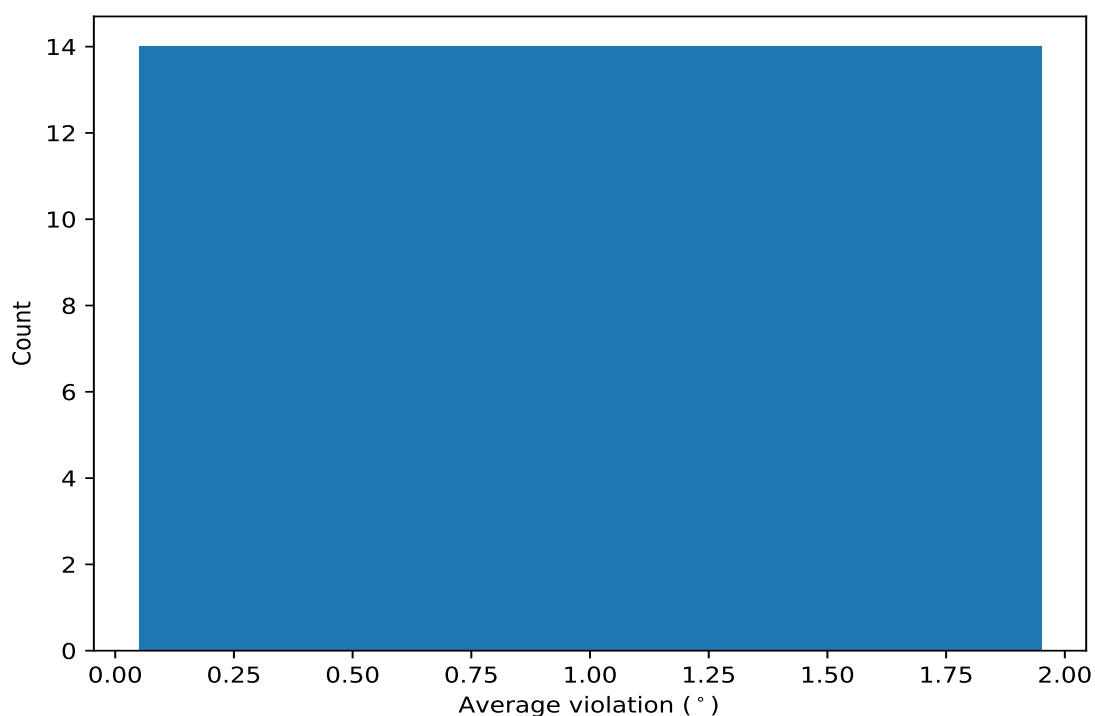
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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.

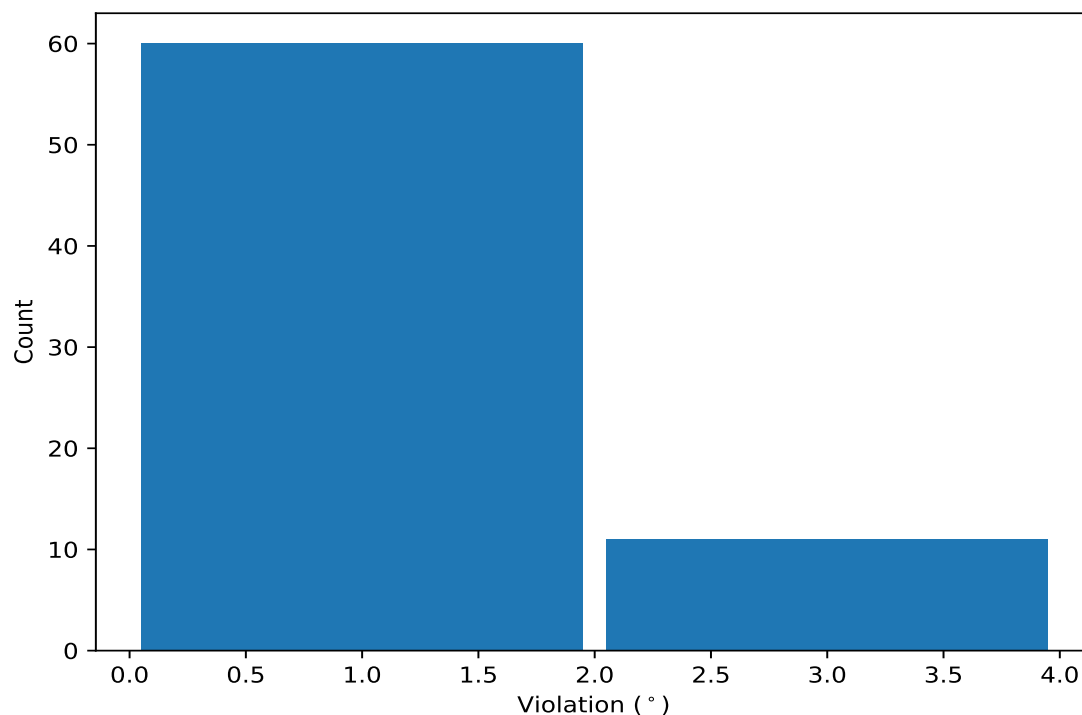
| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|--------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 11                  | 1.9  | 0.44            | 1.89   |
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 8                   | 1.55 | 0.6             | 1.23   |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 8                   | 1.32 | 0.13            | 1.36   |
| (1,32) | 1:227:C:VAL:N | 1:227:C:VAL:CA | 1:227:C:VAL:C  | 1:228:C:ALA:N | 7                   | 1.63 | 0.45            | 1.95   |
| (1,16) | 1:219:C:THR:N | 1:219:C:THR:CA | 1:219:C:THR:C  | 1:220:C:VAL:N | 6                   | 1.55 | 0.34            | 1.44   |
| (1,3)  | 1:212:C:SER:C | 1:213:C:GLY:N  | 1:213:C:GLY:CA | 1:213:C:GLY:C | 3                   | 1.5  | 0.39            | 1.41   |
| (1,50) | 1:236:C:LEU:N | 1:236:C:LEU:CA | 1:236:C:LEU:C  | 1:237:C:TRP:N | 3                   | 1.49 | 0.13            | 1.41   |
| (1,6)  | 1:214:C:ILE:N | 1:214:C:ILE:CA | 1:214:C:ILE:C  | 1:215:C:ILE:N | 3                   | 1.46 | 0.11            | 1.43   |
| (1,8)  | 1:215:C:ILE:N | 1:215:C:ILE:CA | 1:215:C:ILE:C  | 1:216:C:ILE:N | 3                   | 1.29 | 0.26            | 1.18   |
| (1,51) | 1:236:C:LEU:C | 1:237:C:TRP:N  | 1:237:C:TRP:CA | 1:237:C:TRP:C | 3                   | 1.13 | 0.05            | 1.1    |
| (1,30) | 1:226:C:ILE:N | 1:226:C:ILE:CA | 1:226:C:ILE:C  | 1:227:C:VAL:N | 2                   | 1.71 | 0.15            | 1.71   |
| (1,4)  | 1:213:C:GLY:N | 1:213:C:GLY:CA | 1:213:C:GLY:C  | 1:214:C:ILE:N | 2                   | 1.26 | 0.22            | 1.26   |
| (1,52) | 1:237:C:TRP:N | 1:237:C:TRP:CA | 1:237:C:TRP:C  | 1:238:C:LYS:N | 2                   | 1.23 | 0.15            | 1.23   |
| (1,36) | 1:229:C:VAL:N | 1:229:C:VAL:CA | 1:229:C:VAL:C  | 1:230:C:PHE:N | 2                   | 1.2  | 0.12            | 1.2    |

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

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

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

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



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

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

| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 9        | 2.67          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 6        | 2.52          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 13       | 2.39          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 8        | 2.36          |
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 3        | 2.35          |
| (1,16) | 1:219:C:THR:N | 1:219:C:THR:CA | 1:219:C:THR:C  | 1:220:C:VAL:N | 15       | 2.27          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 11       | 2.15          |
| (1,32) | 1:227:C:VAL:N | 1:227:C:VAL:CA | 1:227:C:VAL:C  | 1:228:C:ALA:N | 8        | 2.14          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 7        | 2.11          |
| (1,3)  | 1:212:C:SER:C | 1:213:C:GLY:N  | 1:213:C:GLY:CA | 1:213:C:GLY:C | 11       | 2.02          |
| (1,32) | 1:227:C:VAL:N | 1:227:C:VAL:CA | 1:227:C:VAL:C  | 1:228:C:ALA:N | 13       | 2.01          |
| (1,32) | 1:227:C:VAL:N | 1:227:C:VAL:CA | 1:227:C:VAL:C  | 1:228:C:ALA:N | 6        | 1.98          |
| (1,32) | 1:227:C:VAL:N | 1:227:C:VAL:CA | 1:227:C:VAL:C  | 1:228:C:ALA:N | 11       | 1.95          |
| (1,29) | 1:225:C:LEU:C | 1:226:C:ILE:N  | 1:226:C:ILE:CA | 1:226:C:ILE:C | 14       | 1.95          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 1        | 1.89          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 5        | 1.88          |
| (1,30) | 1:226:C:ILE:N | 1:226:C:ILE:CA | 1:226:C:ILE:C  | 1:227:C:VAL:N | 3        | 1.86          |
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 15       | 1.76          |
| (1,50) | 1:236:C:LEU:N | 1:236:C:LEU:CA | 1:236:C:LEU:C  | 1:237:C:TRP:N | 4        | 1.68          |
| (1,8)  | 1:215:C:ILE:N | 1:215:C:ILE:CA | 1:215:C:ILE:C  | 1:216:C:ILE:N | 11       | 1.65          |
| (1,16) | 1:219:C:THR:N | 1:219:C:THR:CA | 1:219:C:THR:C  | 1:220:C:VAL:N | 4        | 1.61          |
| (1,6)  | 1:214:C:ILE:N | 1:214:C:ILE:CA | 1:214:C:ILE:C  | 1:215:C:ILE:N | 12       | 1.61          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 10       | 1.56          |
| (1,30) | 1:226:C:ILE:N | 1:226:C:ILE:CA | 1:226:C:ILE:C  | 1:227:C:VAL:N | 9        | 1.56          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 12       | 1.55          |
| (1,28) | 1:225:C:LEU:N | 1:225:C:LEU:CA | 1:225:C:LEU:C  | 1:226:C:ILE:N | 14       | 1.53          |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 3        | 1.51          |
| (1,4)  | 1:213:C:GLY:N | 1:213:C:GLY:CA | 1:213:C:GLY:C  | 1:214:C:ILE:N | 11       | 1.48          |
| (1,16) | 1:219:C:THR:N | 1:219:C:THR:CA | 1:219:C:THR:C  | 1:220:C:VAL:N | 12       | 1.45          |
| (1,6)  | 1:214:C:ILE:N | 1:214:C:ILE:CA | 1:214:C:ILE:C  | 1:215:C:ILE:N | 2        | 1.43          |
| (1,16) | 1:219:C:THR:N | 1:219:C:THR:CA | 1:219:C:THR:C  | 1:220:C:VAL:N | 3        | 1.42          |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 1        | 1.42          |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 10       | 1.42          |
| (1,50) | 1:236:C:LEU:N | 1:236:C:LEU:CA | 1:236:C:LEU:C  | 1:237:C:TRP:N | 5        | 1.41          |
| (1,3)  | 1:212:C:SER:C | 1:213:C:GLY:N  | 1:213:C:GLY:CA | 1:213:C:GLY:C | 10       | 1.41          |
| (1,50) | 1:236:C:LEU:N | 1:236:C:LEU:CA | 1:236:C:LEU:C  | 1:237:C:TRP:N | 11       | 1.39          |
| (1,52) | 1:237:C:TRP:N | 1:237:C:TRP:CA | 1:237:C:TRP:C  | 1:238:C:LYS:N | 4        | 1.37          |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 15       | 1.37          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 2        | 1.36          |
| (1,6)  | 1:214:C:ILE:N | 1:214:C:ILE:CA | 1:214:C:ILE:C  | 1:215:C:ILE:N | 4        | 1.35          |
| (1,19) | 1:220:C:VAL:C | 1:221:C:ALA:N  | 1:221:C:ALA:CA | 1:221:C:ALA:C | 13       | 1.34          |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 7        | 1.34          |
| (1,36) | 1:229:C:VAL:N | 1:229:C:VAL:CA | 1:229:C:VAL:C  | 1:230:C:PHE:N | 4        | 1.32          |
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 1        | 1.31          |
| (1,16) | 1:219:C:THR:N | 1:219:C:THR:CA | 1:219:C:THR:C  | 1:220:C:VAL:N | 13       | 1.28          |
| (1,16) | 1:219:C:THR:N | 1:219:C:THR:CA | 1:219:C:THR:C  | 1:220:C:VAL:N | 14       | 1.26          |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 4        | 1.23          |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 8        | 1.22          |
| (1,51) | 1:236:C:LEU:C | 1:237:C:TRP:N  | 1:237:C:TRP:CA | 1:237:C:TRP:C | 9        | 1.2           |
| (1,38) | 1:230:C:PHE:N | 1:230:C:PHE:CA | 1:230:C:PHE:C  | 1:231:C:VAL:N | 4        | 1.18          |
| (1,8)  | 1:215:C:ILE:N | 1:215:C:ILE:CA | 1:215:C:ILE:C  | 1:216:C:ILE:N | 9        | 1.18          |
| (1,5)  | 1:213:C:GLY:C | 1:214:C:ILE:N  | 1:214:C:ILE:CA | 1:214:C:ILE:C | 11       | 1.18          |
| (1,49) | 1:235:C:LEU:C | 1:236:C:LEU:N  | 1:236:C:LEU:CA | 1:236:C:LEU:C | 6        | 1.17          |
| (1,32) | 1:227:C:VAL:N | 1:227:C:VAL:CA | 1:227:C:VAL:C  | 1:228:C:ALA:N | 1        | 1.15          |
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 13       | 1.14          |
| (1,54) | 1:240:C:VAL:N | 1:240:C:VAL:CA | 1:240:C:VAL:C  | 1:241:C:LEU:N | 11       | 1.13          |
| (1,32) | 1:227:C:VAL:N | 1:227:C:VAL:CA | 1:227:C:VAL:C  | 1:228:C:ALA:N | 12       | 1.12          |
| (1,33) | 1:227:C:VAL:C | 1:228:C:ALA:N  | 1:228:C:ALA:CA | 1:228:C:ALA:C | 14       | 1.11          |
| (1,51) | 1:236:C:LEU:C | 1:237:C:TRP:N  | 1:237:C:TRP:CA | 1:237:C:TRP:C | 3        | 1.1           |
| (1,51) | 1:236:C:LEU:C | 1:237:C:TRP:N  | 1:237:C:TRP:CA | 1:237:C:TRP:C | 4        | 1.09          |
| (1,52) | 1:237:C:TRP:N | 1:237:C:TRP:CA | 1:237:C:TRP:C  | 1:238:C:LYS:N | 12       | 1.08          |
| (1,36) | 1:229:C:VAL:N | 1:229:C:VAL:CA | 1:229:C:VAL:C  | 1:230:C:PHE:N | 9        | 1.08          |
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 10       | 1.08          |
| (1,32) | 1:227:C:VAL:N | 1:227:C:VAL:CA | 1:227:C:VAL:C  | 1:228:C:ALA:N | 7        | 1.07          |
| (1,9)  | 1:215:C:ILE:C | 1:216:C:ILE:N  | 1:216:C:ILE:CA | 1:216:C:ILE:C | 12       | 1.07          |

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| Key    | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|--------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,3)  | 1:212:C:SER:C | 1:213:C:GLY:N  | 1:213:C:GLY:CA | 1:213:C:GLY:C | 9        | 1.07          |
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 14       | 1.06          |
| (1,17) | 1:219:C:THR:C | 1:220:C:VAL:N  | 1:220:C:VAL:CA | 1:220:C:VAL:C | 13       | 1.05          |
| (1,31) | 1:226:C:ILE:C | 1:227:C:VAL:N  | 1:227:C:VAL:CA | 1:227:C:VAL:C | 8        | 1.04          |
| (1,8)  | 1:215:C:ILE:N | 1:215:C:ILE:CA | 1:215:C:ILE:C  | 1:216:C:ILE:N | 2        | 1.04          |
| (1,4)  | 1:213:C:GLY:N | 1:213:C:GLY:CA | 1:213:C:GLY:C  | 1:214:C:ILE:N | 10       | 1.04          |