



Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 04:39 AM EDT

PDB ID : 2AN7
BMRB ID : 4792
Title : Solution structure of the bacterial antidote ParD
Authors : Oberer, M.; Zangger, K.; Gruber, K.; Keller, W.
Deposited on : 2005-08-11

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

We welcome your comments at 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>.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.33

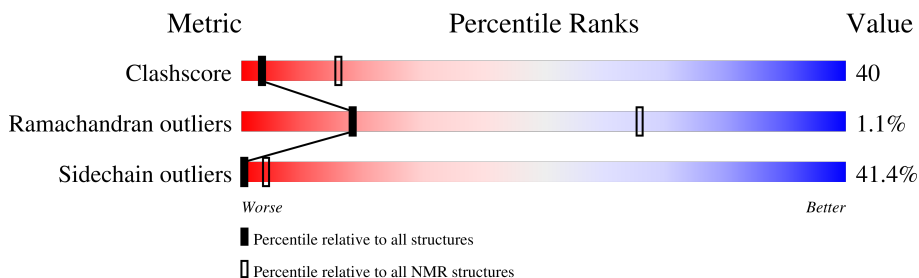
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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 (#Entries) | NMR archive (#Entries) |
|-----------------------|--------------------------|------------------------|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

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 ≥ 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 | 83 | |
| 1 | B | 83 | |

2 Ensemble composition and analysis

This entry contains 24 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:2-A:35, B:102-B:135 (68) | 0.54 | 1 |
| 2 | A:39-A:55 (17) | 2.35 | 24 |

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, 4, 7, 8, 9, 12, 14, 15, 17, 18, 19, 21, 22, 23, 24 |
| 2 | 2, 3, 10, 11, 13, 16, 20 |
| 3 | 5, 6 |

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2556 atoms, of which 1282 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein parD.

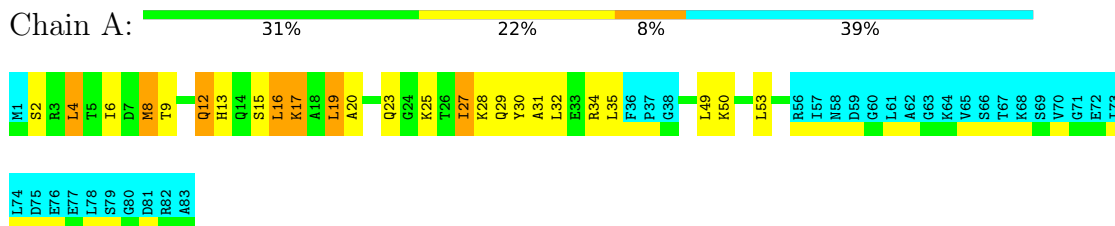
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| | | | Total | C | H | N | O | S | |
| 1 | A | 83 | 1278 | 391 | 641 | 113 | 130 | 3 | 0 |
| 1 | B | 83 | 1278 | 391 | 641 | 113 | 130 | 3 | 0 |

4 Residue-property plots [i](#)

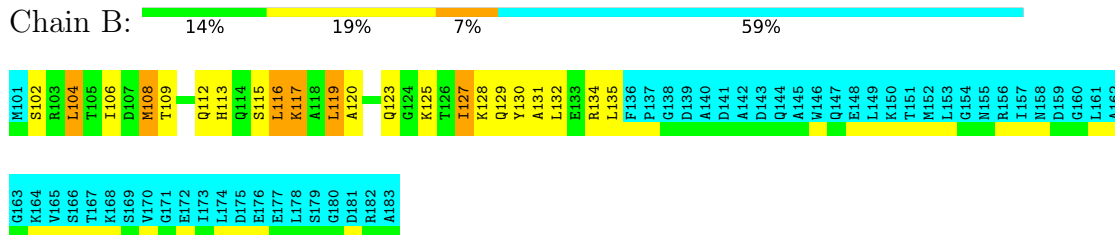
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Protein parD



- Molecule 1: Protein parD

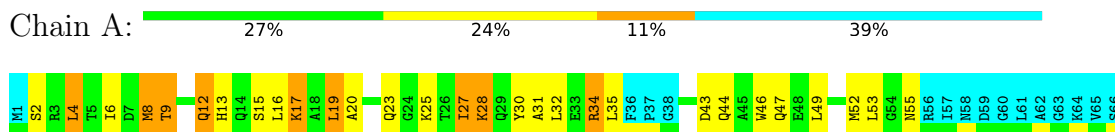


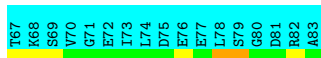
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

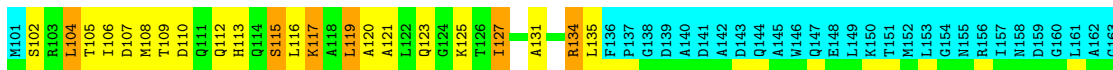
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Protein parD



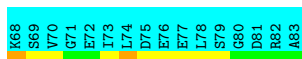
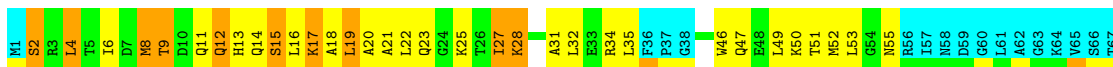


- Molecule 1: Protein parD



4.2.2 Score per residue for model 2

- Molecule 1: Protein parD

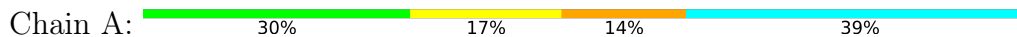


- Molecule 1: Protein parD

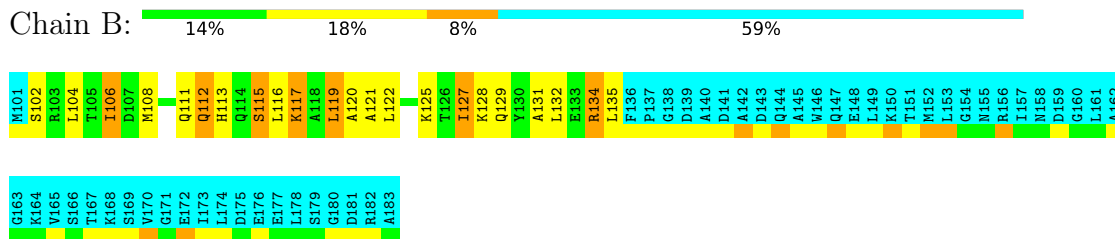


4.2.3 Score per residue for model 3

- Molecule 1: Protein parD

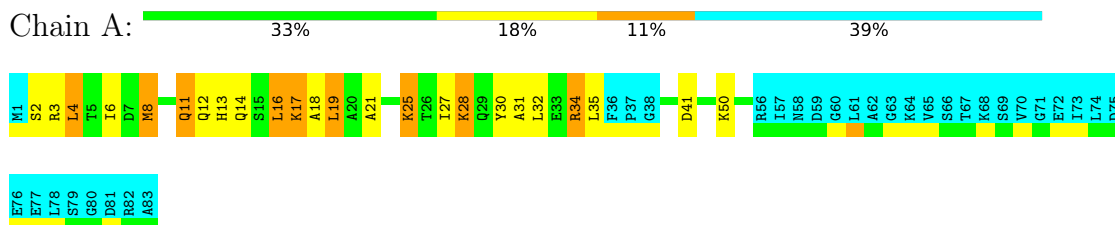


- Molecule 1: Protein parD

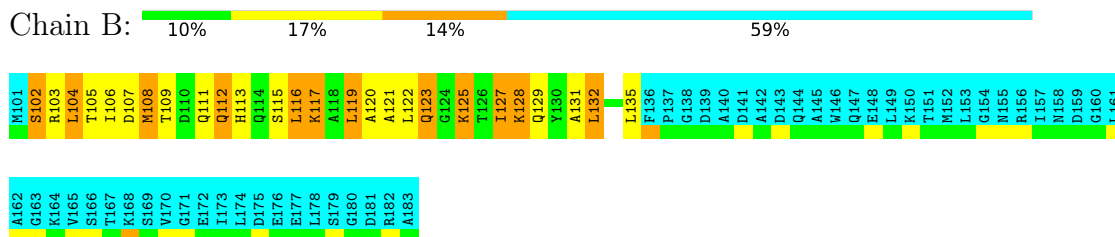


4.2.4 Score per residue for model 4

- Molecule 1: Protein parD

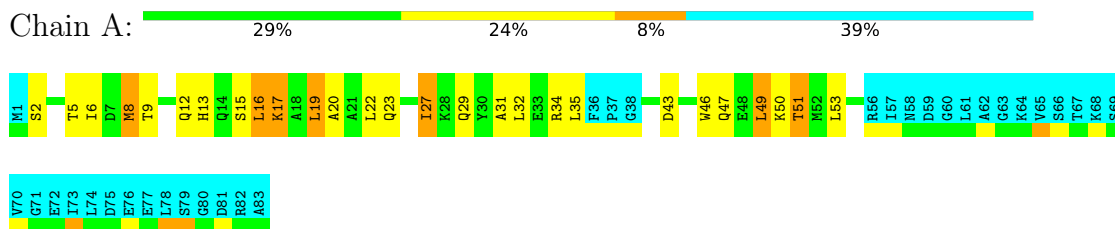


- Molecule 1: Protein parD

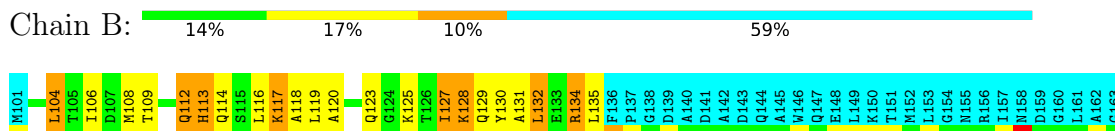


4.2.5 Score per residue for model 5

- Molecule 1: Protein parD



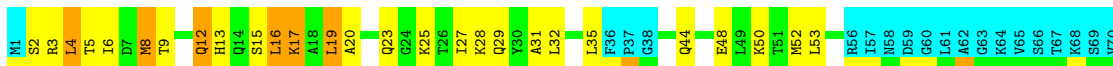
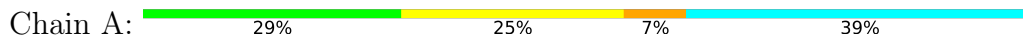
- Molecule 1: Protein parD



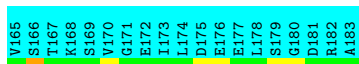


4.2.6 Score per residue for model 6

- Molecule 1: Protein parD

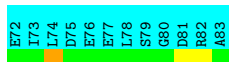
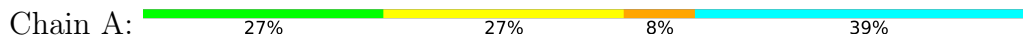


- Molecule 1: Protein parD

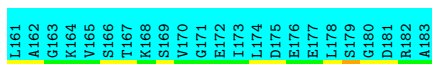
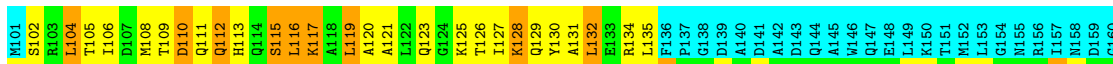


4.2.7 Score per residue for model 7

- Molecule 1: Protein parD

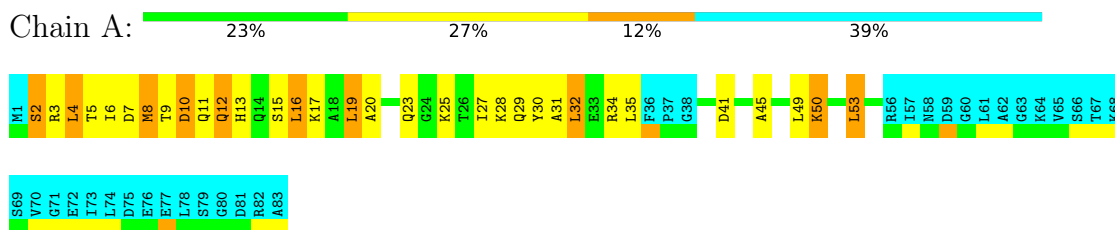


- Molecule 1: Protein parD

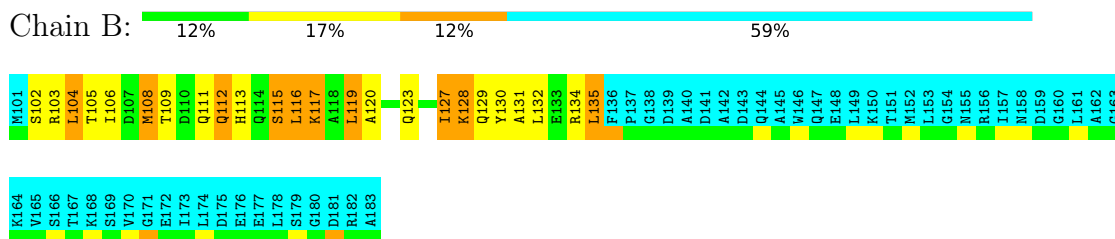


4.2.8 Score per residue for model 8

- Molecule 1: Protein parD

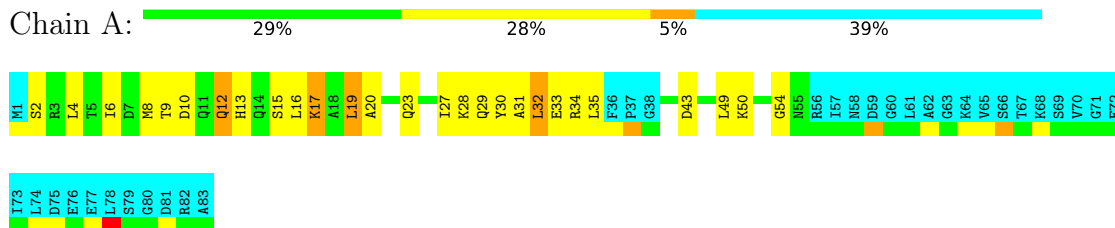


- Molecule 1: Protein parD

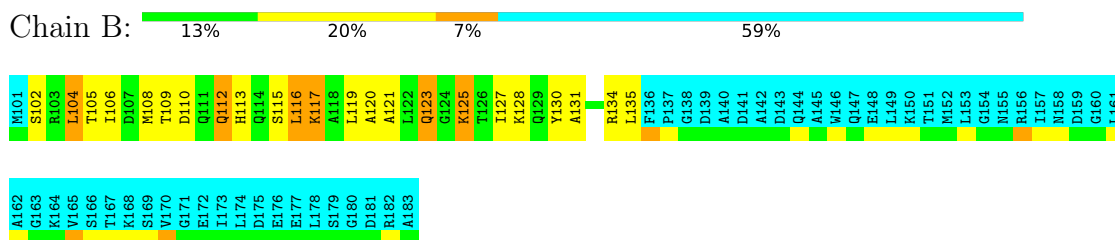


4.2.9 Score per residue for model 9

- Molecule 1: Protein parD

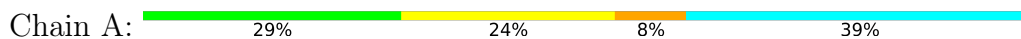


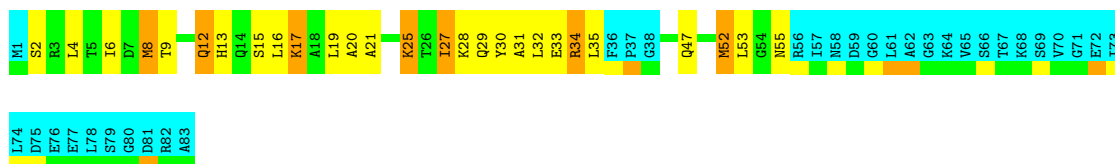
- Molecule 1: Protein parD



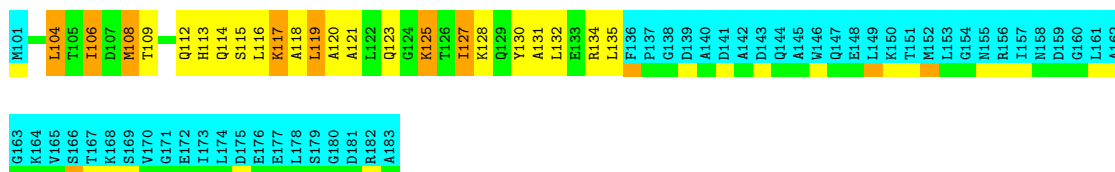
4.2.10 Score per residue for model 10

- Molecule 1: Protein parD



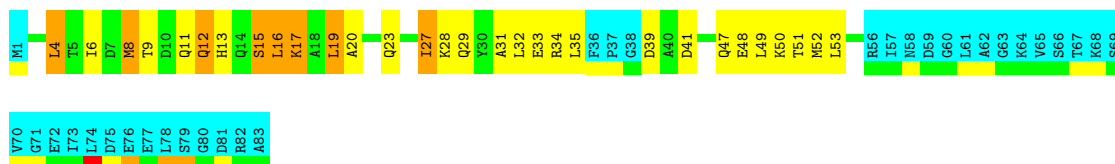
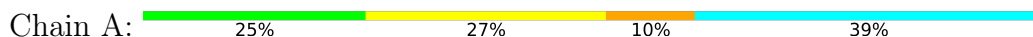


- Molecule 1: Protein parD

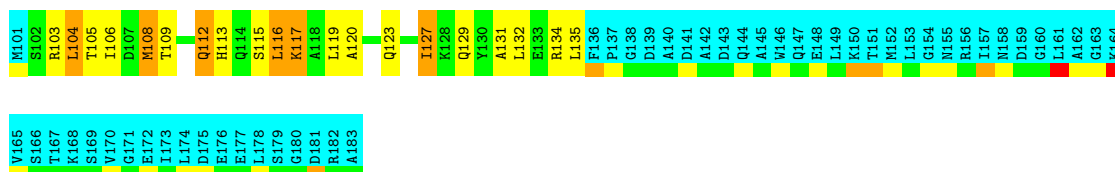


4.2.11 Score per residue for model 11

- Molecule 1: Protein parD

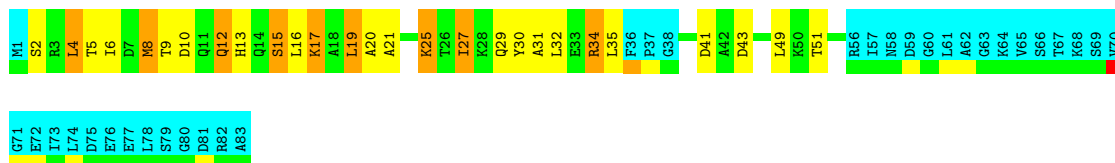
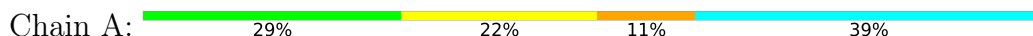


- Molecule 1: Protein parD

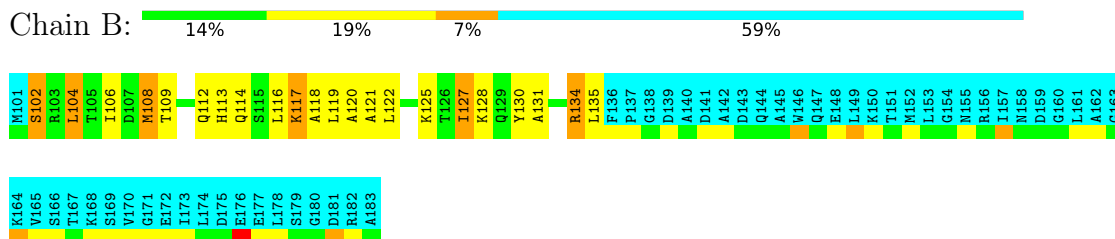


4.2.12 Score per residue for model 12

- Molecule 1: Protein parD

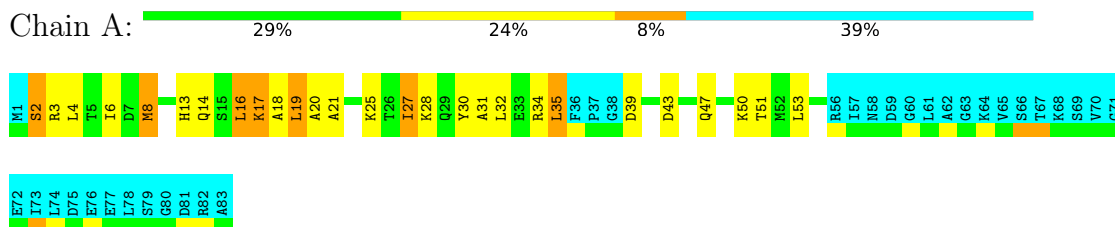


- Molecule 1: Protein parD

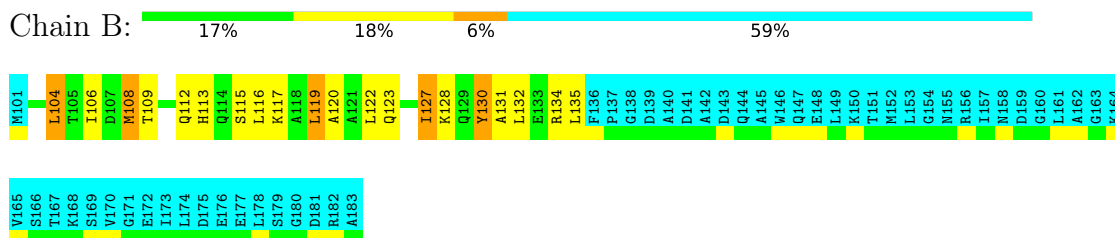


4.2.13 Score per residue for model 13

- Molecule 1: Protein parD

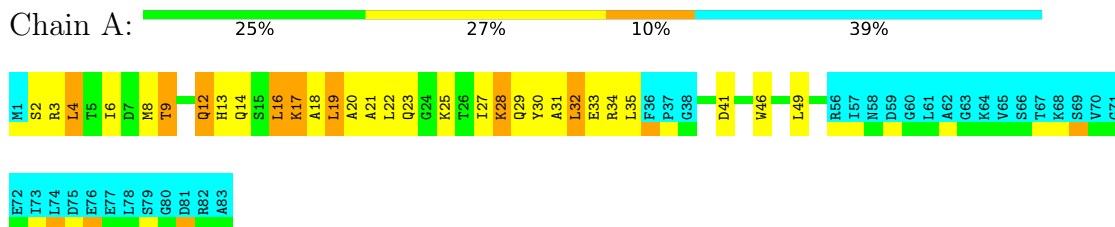


- Molecule 1: Protein parD



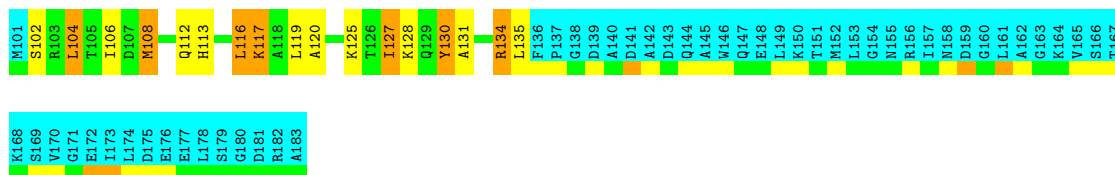
4.2.14 Score per residue for model 14

- Molecule 1: Protein parD



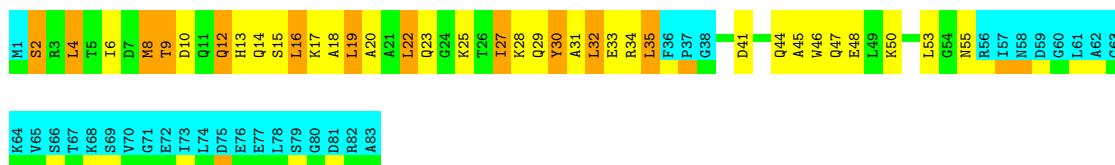
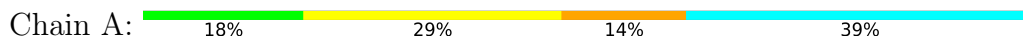
- Molecule 1: Protein parD



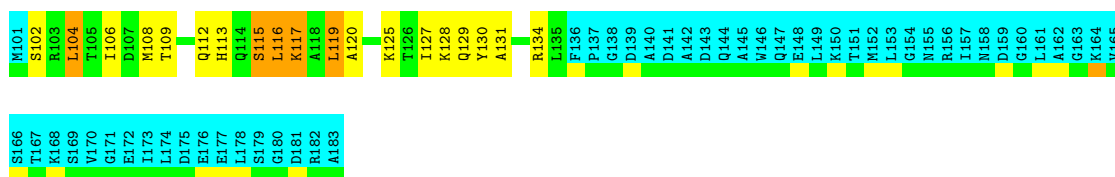


4.2.15 Score per residue for model 15

- Molecule 1: Protein parD

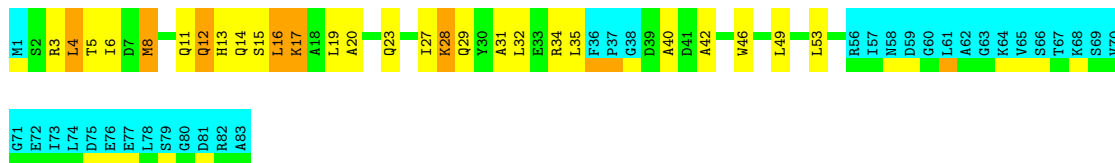
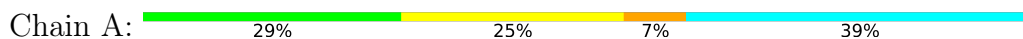


- Molecule 1: Protein parD

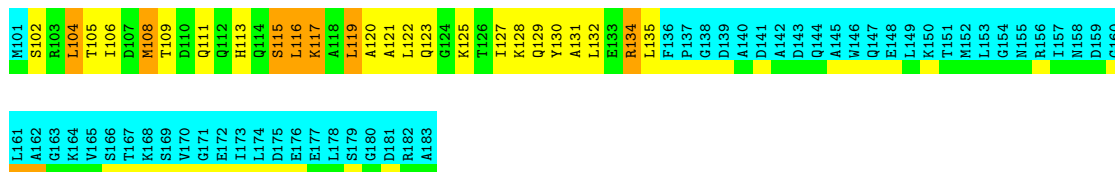


4.2.16 Score per residue for model 16

- Molecule 1: Protein parD

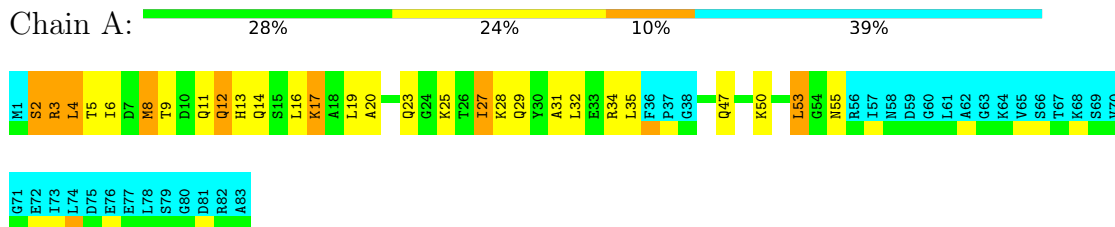


- Molecule 1: Protein parD

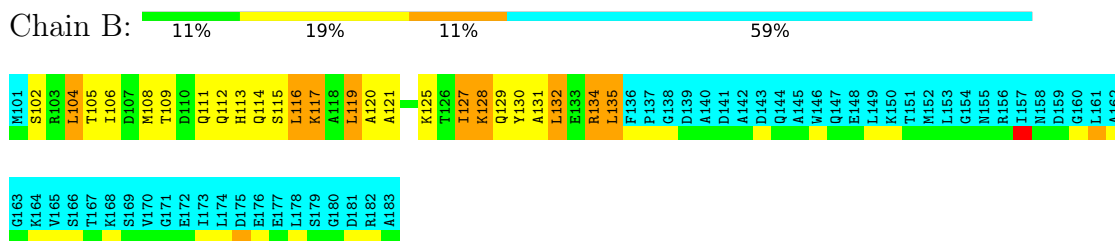


4.2.17 Score per residue for model 17

- Molecule 1: Protein parD

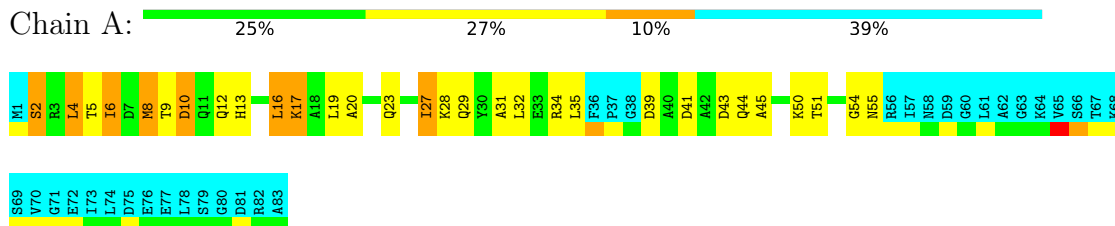


- Molecule 1: Protein parD

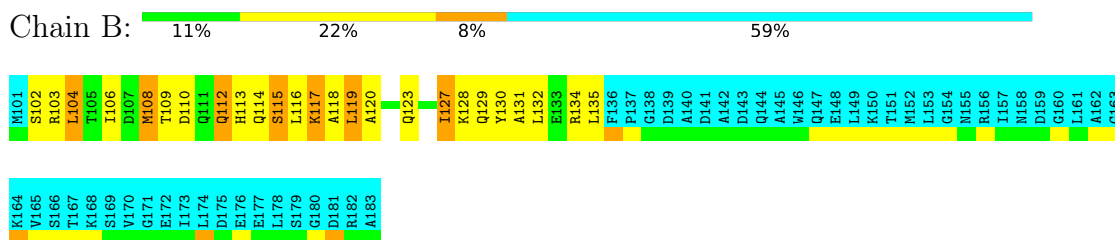


4.2.18 Score per residue for model 18

- Molecule 1: Protein parD

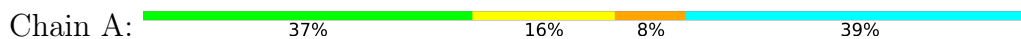


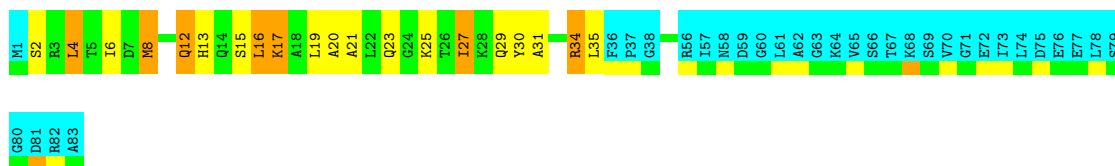
- Molecule 1: Protein parD



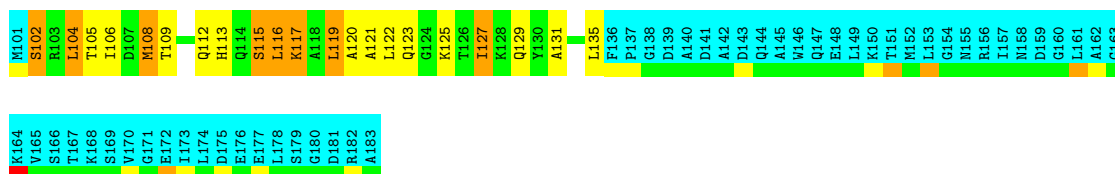
4.2.19 Score per residue for model 19

- Molecule 1: Protein parD



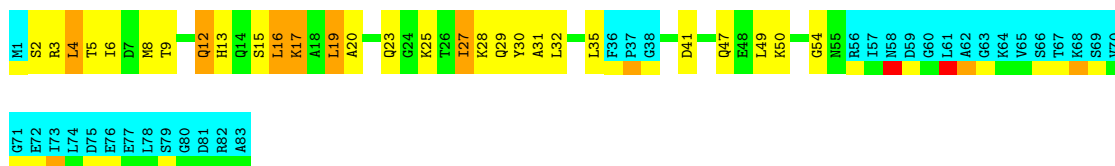
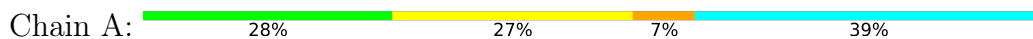


- Molecule 1: Protein parD

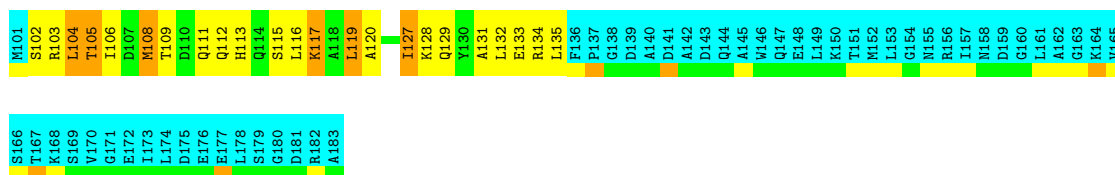


4.2.20 Score per residue for model 20

- Molecule 1: Protein parD

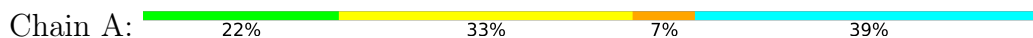


- Molecule 1: Protein parD




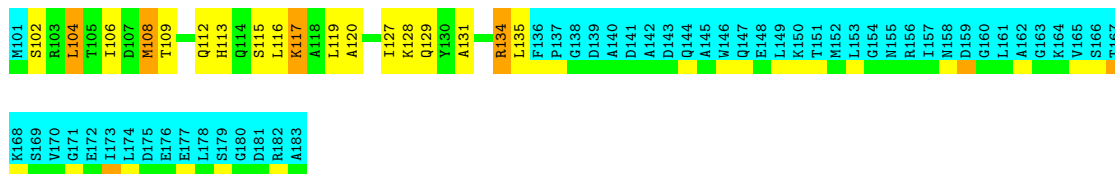
4.2.21 Score per residue for model 21

- Molecule 1: Protein parD



- Molecule 1: Protein parD

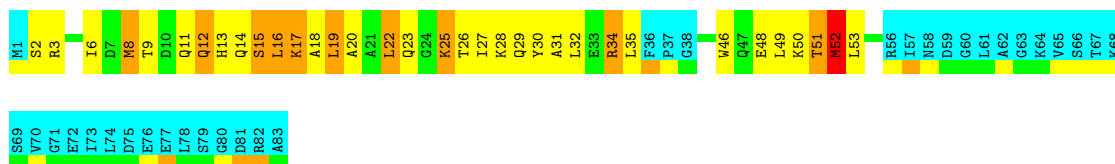
Chain B: 



4.2.22 Score per residue for model 22

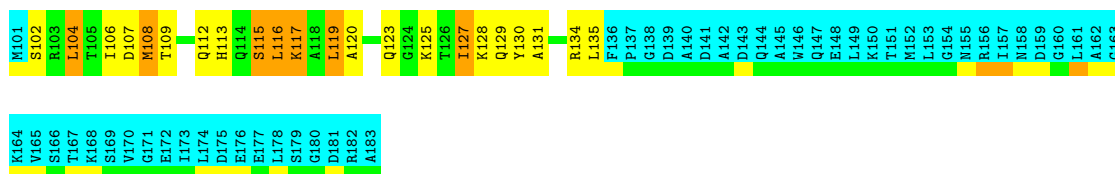
- Molecule 1: Protein parD

Chain A: 




- Molecule 1: Protein parD

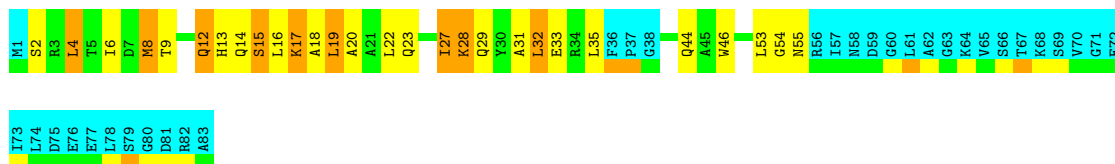
Chain B: 



4.2.23 Score per residue for model 23

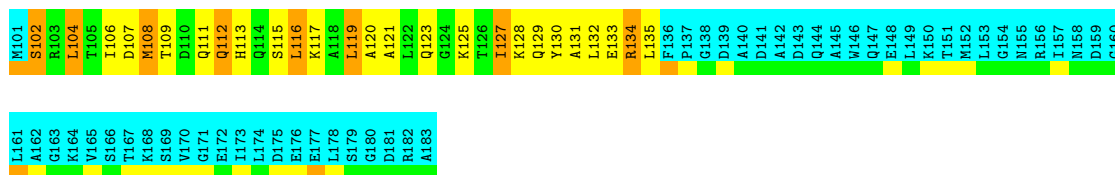
- Molecule 1: Protein parD

Chain A: 



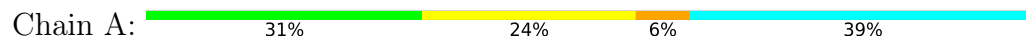
- Molecule 1: Protein parD

Chain B: 

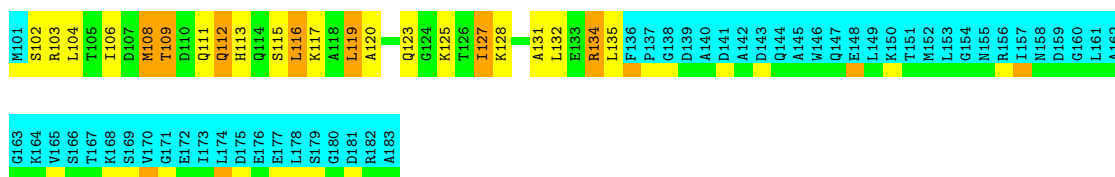


4.2.24 Score per residue for model 24

- Molecule 1: Protein parD



- Molecule 1: Protein parD



5 Refinement protocol and experimental data overview

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

Of the 150 calculated structures, 24 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 |
|---------------|--------------------|---------|
| CNS | refinement | 1.1 |
| CNS | structure solution | 1.1 |

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

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1712 |
| Number of shifts mapped to atoms | 1712 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 77% |

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 402 | 406 | 405 | 37±6 |
| 1 | B | 270 | 287 | 286 | 35±7 |
| All | All | 16128 | 16632 | 16584 | 1324 |

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 40.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:104:LEU:HD21 | 1:B:106:ILE:HD11 | 1.04 | 1.20 | 18 | 10 |
| 1:A:4:LEU:HD21 | 1:A:6:ILE:HD11 | 0.99 | 1.34 | 11 | 11 |
| 1:A:16:LEU:HD13 | 1:A:17:LYS:N | 0.91 | 1.81 | 11 | 4 |
| 1:A:17:LYS:N | 1:A:17:LYS:HD3 | 0.91 | 1.78 | 13 | 2 |
| 1:A:32:LEU:HB2 | 1:B:106:ILE:HD11 | 0.89 | 1.44 | 7 | 4 |
| 1:A:6:ILE:HD12 | 1:B:106:ILE:HD12 | 0.89 | 1.45 | 14 | 9 |
| 1:B:116:LEU:HD22 | 1:B:117:LYS:N | 0.89 | 1.83 | 23 | 3 |
| 1:B:116:LEU:HD12 | 1:B:117:LYS:N | 0.89 | 1.82 | 3 | 3 |
| 1:B:117:LYS:N | 1:B:117:LYS:HD3 | 0.89 | 1.81 | 12 | 1 |
| 1:A:27:ILE:HD12 | 1:A:31:ALA:HB2 | 0.88 | 1.44 | 23 | 4 |
| 1:A:27:ILE:CD1 | 1:A:31:ALA:HB2 | 0.88 | 1.98 | 19 | 7 |
| 1:A:19:LEU:HD11 | 1:A:30:TYR:CZ | 0.87 | 2.04 | 13 | 3 |
| 1:A:31:ALA:HB1 | 1:B:135:LEU:HD22 | 0.86 | 1.44 | 4 | 12 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:35:LEU:HD22 | 1:B:131:ALA:HB1 | 0.86 | 1.48 | 8 | 10 |
| 1:B:116:LEU:HD13 | 1:B:117:LYS:N | 0.86 | 1.86 | 8 | 3 |
| 1:A:27:ILE:HD11 | 1:B:104:LEU:HD22 | 0.84 | 1.47 | 18 | 8 |
| 1:A:19:LEU:O | 1:A:22:LEU:HD23 | 0.84 | 1.70 | 22 | 2 |
| 1:B:116:LEU:HD11 | 1:B:127:ILE:CD1 | 0.83 | 2.04 | 2 | 4 |
| 1:A:4:LEU:HD22 | 1:B:127:ILE:HD11 | 0.83 | 1.51 | 7 | 8 |
| 1:B:127:ILE:CD1 | 1:B:131:ALA:HB2 | 0.82 | 2.04 | 12 | 8 |
| 1:A:16:LEU:HD22 | 1:A:17:LYS:N | 0.81 | 1.89 | 15 | 2 |
| 1:A:4:LEU:HD22 | 1:B:117:LYS:NZ | 0.81 | 1.90 | 12 | 1 |
| 1:A:16:LEU:HD21 | 1:A:27:ILE:CD1 | 0.81 | 2.05 | 16 | 6 |
| 1:A:17:LYS:NZ | 1:B:104:LEU:HD22 | 0.81 | 1.91 | 13 | 1 |
| 1:A:49:LEU:HD12 | 1:A:50:LYS:N | 0.80 | 1.91 | 8 | 1 |
| 1:A:16:LEU:HD21 | 1:A:27:ILE:HD12 | 0.80 | 1.52 | 20 | 5 |
| 1:A:31:ALA:HB1 | 1:B:135:LEU:CD2 | 0.80 | 2.07 | 5 | 9 |
| 1:A:13:HIS:O | 1:A:17:LYS:HB2 | 0.79 | 1.75 | 24 | 18 |
| 1:B:116:LEU:HD21 | 1:B:127:ILE:CD1 | 0.79 | 2.08 | 7 | 4 |
| 1:A:27:ILE:HD11 | 1:A:31:ALA:HB2 | 0.79 | 1.54 | 19 | 2 |
| 1:B:116:LEU:HD13 | 1:B:127:ILE:CD1 | 0.79 | 2.07 | 3 | 2 |
| 1:A:16:LEU:HD11 | 1:A:27:ILE:CD1 | 0.79 | 2.08 | 8 | 2 |
| 1:A:6:ILE:HD11 | 1:B:132:LEU:HB2 | 0.78 | 1.56 | 16 | 2 |
| 1:A:35:LEU:HG | 1:B:135:LEU:HD21 | 0.78 | 1.54 | 14 | 3 |
| 1:A:9:THR:HG22 | 1:A:12:GLN:HG2 | 0.77 | 1.56 | 22 | 1 |
| 1:B:113:HIS:O | 1:B:117:LYS:HB2 | 0.77 | 1.78 | 24 | 21 |
| 1:B:115:SER:O | 1:B:119:LEU:HD12 | 0.77 | 1.79 | 24 | 16 |
| 1:A:5:THR:OG1 | 1:B:105:THR:HG23 | 0.77 | 1.80 | 8 | 1 |
| 1:A:35:LEU:CD2 | 1:B:131:ALA:HB1 | 0.76 | 2.10 | 8 | 6 |
| 1:A:27:ILE:HG13 | 1:A:31:ALA:HB2 | 0.76 | 1.58 | 20 | 11 |
| 1:B:116:LEU:CD1 | 1:B:127:ILE:HD12 | 0.75 | 2.10 | 21 | 1 |
| 1:A:35:LEU:O | 1:B:116:LEU:HD21 | 0.75 | 1.81 | 10 | 8 |
| 1:A:15:SER:O | 1:A:19:LEU:HD12 | 0.75 | 1.81 | 23 | 11 |
| 1:A:20:ALA:HB1 | 1:A:27:ILE:HA | 0.75 | 1.59 | 15 | 6 |
| 1:A:8:MET:HE1 | 1:B:135:LEU:HD13 | 0.74 | 1.57 | 10 | 3 |
| 1:B:104:LEU:HD11 | 1:B:106:ILE:CG1 | 0.74 | 2.12 | 18 | 7 |
| 1:A:17:LYS:HG2 | 1:A:27:ILE:HG21 | 0.74 | 1.58 | 15 | 2 |
| 1:B:104:LEU:CD2 | 1:B:106:ILE:HD11 | 0.73 | 2.08 | 18 | 3 |
| 1:A:16:LEU:HD21 | 1:B:135:LEU:O | 0.73 | 1.83 | 13 | 3 |
| 1:B:116:LEU:HD13 | 1:B:127:ILE:HD12 | 0.73 | 1.59 | 21 | 2 |
| 1:A:8:MET:CE | 1:B:135:LEU:HD13 | 0.73 | 2.14 | 5 | 3 |
| 1:B:117:LYS:HG2 | 1:B:127:ILE:HG21 | 0.73 | 1.58 | 23 | 3 |
| 1:B:127:ILE:HD11 | 1:B:131:ALA:HB2 | 0.73 | 1.59 | 10 | 5 |
| 1:A:16:LEU:HD12 | 1:A:30:TYR:CE2 | 0.73 | 2.18 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:4:LEU:CD2 | 1:A:6:ILE:HD11 | 0.72 | 2.14 | 10 | 7 |
| 1:A:16:LEU:HD23 | 1:B:135:LEU:HB3 | 0.72 | 1.61 | 24 | 1 |
| 1:A:20:ALA:CB | 1:A:27:ILE:HA | 0.72 | 2.15 | 15 | 14 |
| 1:A:19:LEU:HD21 | 1:A:30:TYR:OH | 0.72 | 1.84 | 4 | 1 |
| 1:B:132:LEU:HA | 1:B:135:LEU:HD12 | 0.72 | 1.62 | 5 | 3 |
| 1:B:127:ILE:HG13 | 1:B:131:ALA:HB2 | 0.72 | 1.61 | 2 | 8 |
| 1:A:16:LEU:HD22 | 1:A:27:ILE:CD1 | 0.71 | 2.15 | 24 | 1 |
| 1:A:16:LEU:HA | 1:A:19:LEU:HD23 | 0.71 | 1.60 | 4 | 4 |
| 1:B:116:LEU:HD21 | 1:B:127:ILE:HD12 | 0.71 | 1.63 | 7 | 3 |
| 1:A:16:LEU:HD13 | 1:B:135:LEU:O | 0.71 | 1.86 | 2 | 1 |
| 1:A:13:HIS:O | 1:A:16:LEU:HD23 | 0.70 | 1.85 | 5 | 3 |
| 1:A:16:LEU:HD23 | 1:A:27:ILE:HD13 | 0.70 | 1.63 | 15 | 1 |
| 1:A:16:LEU:HD21 | 1:A:31:ALA:HB2 | 0.70 | 1.62 | 2 | 3 |
| 1:B:116:LEU:HD11 | 1:B:127:ILE:HD11 | 0.70 | 1.63 | 8 | 4 |
| 1:A:35:LEU:HD13 | 1:B:108:MET:CE | 0.70 | 2.17 | 14 | 3 |
| 1:B:119:LEU:HD11 | 1:B:130:TYR:CZ | 0.69 | 2.21 | 17 | 1 |
| 1:B:113:HIS:O | 1:B:117:LYS:CD | 0.69 | 2.40 | 5 | 1 |
| 1:A:16:LEU:C | 1:A:16:LEU:HD22 | 0.69 | 2.07 | 7 | 4 |
| 1:A:8:MET:SD | 1:B:104:LEU:HD23 | 0.69 | 2.27 | 19 | 4 |
| 1:A:13:HIS:CD2 | 1:A:17:LYS:HG2 | 0.69 | 2.23 | 19 | 2 |
| 1:A:5:THR:C | 1:A:6:ILE:HD13 | 0.69 | 2.08 | 3 | 1 |
| 1:A:16:LEU:HD22 | 1:A:27:ILE:HD11 | 0.69 | 1.65 | 24 | 1 |
| 1:B:116:LEU:CD1 | 1:B:127:ILE:HD13 | 0.68 | 2.17 | 13 | 2 |
| 1:A:28:LYS:O | 1:A:32:LEU:HD12 | 0.68 | 1.87 | 23 | 2 |
| 1:B:128:LYS:O | 1:B:132:LEU:HD12 | 0.68 | 1.89 | 4 | 2 |
| 1:A:6:ILE:CD1 | 1:B:106:ILE:HD12 | 0.68 | 2.18 | 14 | 4 |
| 1:A:32:LEU:HA | 1:A:35:LEU:HD12 | 0.68 | 1.66 | 21 | 2 |
| 1:A:8:MET:SD | 1:B:132:LEU:HD13 | 0.68 | 2.29 | 20 | 1 |
| 1:A:35:LEU:O | 1:B:116:LEU:HD11 | 0.67 | 1.90 | 12 | 3 |
| 1:B:104:LEU:HD12 | 1:B:105:THR:N | 0.67 | 2.05 | 7 | 1 |
| 1:B:113:HIS:CD2 | 1:B:117:LYS:HD3 | 0.67 | 2.25 | 5 | 2 |
| 1:A:17:LYS:CD | 1:A:27:ILE:HD13 | 0.67 | 2.20 | 13 | 2 |
| 1:A:16:LEU:HD22 | 1:B:135:LEU:HB3 | 0.66 | 1.65 | 2 | 5 |
| 1:B:116:LEU:HD22 | 1:B:116:LEU:C | 0.66 | 2.11 | 11 | 5 |
| 1:A:4:LEU:HD11 | 1:A:6:ILE:CG1 | 0.66 | 2.19 | 15 | 4 |
| 1:A:35:LEU:HD11 | 1:B:106:ILE:HD13 | 0.66 | 1.65 | 14 | 3 |
| 1:A:32:LEU:HD13 | 1:B:108:MET:SD | 0.66 | 2.31 | 18 | 2 |
| 1:B:116:LEU:HD13 | 1:B:117:LYS:H | 0.66 | 1.50 | 9 | 3 |
| 1:A:16:LEU:HD22 | 1:A:16:LEU:O | 0.66 | 1.91 | 11 | 4 |
| 1:A:35:LEU:HD13 | 1:A:35:LEU:N | 0.66 | 2.05 | 15 | 1 |
| 1:A:19:LEU:HD11 | 1:A:30:TYR:CE1 | 0.66 | 2.25 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:104:LEU:HD11 | 1:B:106:ILE:HG13 | 0.66 | 1.66 | 15 | 4 |
| 1:A:16:LEU:CD2 | 1:A:27:ILE:HD13 | 0.66 | 2.21 | 15 | 1 |
| 1:A:6:ILE:HD12 | 1:B:106:ILE:HD13 | 0.66 | 1.66 | 15 | 1 |
| 1:A:35:LEU:HD21 | 1:B:131:ALA:CB | 0.65 | 2.22 | 13 | 1 |
| 1:A:32:LEU:HD11 | 1:B:107:ASP:O | 0.65 | 1.91 | 22 | 2 |
| 1:A:16:LEU:HD22 | 1:A:16:LEU:C | 0.65 | 2.11 | 11 | 2 |
| 1:A:16:LEU:HD13 | 1:A:30:TYR:CE2 | 0.65 | 2.27 | 19 | 3 |
| 1:A:16:LEU:HD23 | 1:A:17:LYS:N | 0.65 | 2.07 | 14 | 1 |
| 1:A:31:ALA:CB | 1:B:135:LEU:HD22 | 0.64 | 2.21 | 4 | 8 |
| 1:A:35:LEU:HD21 | 1:B:135:LEU:HG | 0.64 | 1.68 | 5 | 3 |
| 1:A:9:THR:HG22 | 1:A:12:GLN:HB2 | 0.64 | 1.67 | 18 | 1 |
| 1:A:8:MET:CE | 1:B:135:LEU:HD12 | 0.63 | 2.23 | 18 | 7 |
| 1:A:16:LEU:CD1 | 1:B:135:LEU:HD13 | 0.63 | 2.23 | 14 | 1 |
| 1:A:16:LEU:CD2 | 1:A:27:ILE:HD12 | 0.63 | 2.23 | 20 | 4 |
| 1:A:35:LEU:HD12 | 1:B:108:MET:CE | 0.63 | 2.24 | 23 | 6 |
| 1:A:6:ILE:HD12 | 1:B:106:ILE:CD1 | 0.63 | 2.23 | 1 | 3 |
| 1:A:35:LEU:HD23 | 1:B:134:ARG:HB3 | 0.63 | 1.70 | 3 | 6 |
| 1:B:116:LEU:HA | 1:B:119:LEU:HD23 | 0.63 | 1.71 | 17 | 1 |
| 1:A:53:LEU:HD12 | 1:A:53:LEU:O | 0.63 | 1.94 | 5 | 1 |
| 1:B:116:LEU:HD13 | 1:B:116:LEU:C | 0.63 | 2.14 | 8 | 1 |
| 1:A:16:LEU:HD21 | 1:A:31:ALA:CB | 0.62 | 2.24 | 2 | 2 |
| 1:A:35:LEU:HD21 | 1:B:135:LEU:CD2 | 0.62 | 2.24 | 11 | 4 |
| 1:A:35:LEU:HD13 | 1:B:108:MET:HE1 | 0.62 | 1.71 | 21 | 3 |
| 1:A:4:LEU:HD11 | 1:A:6:ILE:HG12 | 0.62 | 1.68 | 17 | 3 |
| 1:A:13:HIS:CD2 | 1:A:17:LYS:HE2 | 0.62 | 2.29 | 19 | 1 |
| 1:A:35:LEU:HD22 | 1:B:131:ALA:HA | 0.62 | 1.70 | 3 | 3 |
| 1:B:127:ILE:HG12 | 1:B:131:ALA:HB2 | 0.62 | 1.71 | 11 | 2 |
| 1:B:135:LEU:N | 1:B:135:LEU:HD13 | 0.62 | 2.10 | 8 | 1 |
| 1:A:31:ALA:O | 1:A:35:LEU:HG | 0.62 | 1.94 | 10 | 8 |
| 1:A:35:LEU:HD12 | 1:B:135:LEU:HD21 | 0.62 | 1.70 | 13 | 1 |
| 1:B:120:ALA:HB1 | 1:B:127:ILE:N | 0.61 | 2.10 | 19 | 23 |
| 1:A:13:HIS:O | 1:A:17:LYS:CB | 0.61 | 2.47 | 23 | 15 |
| 1:A:35:LEU:HD22 | 1:B:116:LEU:HD22 | 0.61 | 1.71 | 13 | 1 |
| 1:B:113:HIS:O | 1:B:117:LYS:HD2 | 0.61 | 1.96 | 10 | 2 |
| 1:B:113:HIS:CD2 | 1:B:117:LYS:HE3 | 0.61 | 2.31 | 12 | 1 |
| 1:A:53:LEU:HD22 | 1:A:53:LEU:N | 0.61 | 2.11 | 8 | 2 |
| 1:A:16:LEU:HD13 | 1:B:135:LEU:HB3 | 0.61 | 1.72 | 8 | 2 |
| 1:A:41:ASP:O | 1:A:45:ALA:HB2 | 0.61 | 1.95 | 8 | 1 |
| 1:B:104:LEU:HD11 | 1:B:106:ILE:CD1 | 0.61 | 2.25 | 19 | 2 |
| 1:A:27:ILE:CD1 | 1:B:104:LEU:HD22 | 0.60 | 2.24 | 18 | 8 |
| 1:B:127:ILE:CG1 | 1:B:131:ALA:HB2 | 0.60 | 2.26 | 6 | 6 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:116:LEU:HD11 | 1:B:127:ILE:HG13 | 0.60 | 1.73 | 15 | 1 |
| 1:A:46:TRP:HA | 1:A:49:LEU:HD23 | 0.60 | 1.73 | 24 | 1 |
| 1:A:53:LEU:H | 1:A:53:LEU:HD13 | 0.60 | 1.56 | 7 | 2 |
| 1:A:35:LEU:HD13 | 1:B:131:ALA:HB1 | 0.60 | 1.72 | 10 | 2 |
| 1:B:113:HIS:O | 1:B:117:LYS:CB | 0.60 | 2.50 | 23 | 15 |
| 1:B:127:ILE:HD12 | 1:B:131:ALA:HB2 | 0.60 | 1.73 | 24 | 5 |
| 1:A:9:THR:HG23 | 1:A:12:GLN:CB | 0.60 | 2.27 | 2 | 5 |
| 1:A:18:ALA:O | 1:A:22:LEU:HD13 | 0.59 | 1.97 | 2 | 2 |
| 1:A:32:LEU:CB | 1:B:106:ILE:HD11 | 0.59 | 2.26 | 4 | 2 |
| 1:A:16:LEU:HD13 | 1:A:17:LYS:H | 0.59 | 1.56 | 6 | 4 |
| 1:B:116:LEU:HD12 | 1:B:116:LEU:O | 0.59 | 1.96 | 15 | 1 |
| 1:A:4:LEU:HD22 | 1:B:117:LYS:HZ2 | 0.59 | 1.57 | 12 | 1 |
| 1:A:35:LEU:HD21 | 1:B:131:ALA:HB1 | 0.59 | 1.74 | 13 | 1 |
| 1:A:20:ALA:HB2 | 1:A:30:TYR:CD1 | 0.59 | 2.33 | 15 | 1 |
| 1:A:35:LEU:CB | 1:B:116:LEU:HD11 | 0.59 | 2.28 | 10 | 1 |
| 1:A:8:MET:HE1 | 1:B:135:LEU:HD12 | 0.59 | 1.75 | 6 | 6 |
| 1:A:14:GLN:O | 1:A:18:ALA:HB3 | 0.59 | 1.97 | 23 | 1 |
| 1:A:27:ILE:CG1 | 1:A:31:ALA:HB2 | 0.59 | 2.27 | 9 | 8 |
| 1:B:106:ILE:N | 1:B:106:ILE:HD13 | 0.59 | 2.12 | 3 | 1 |
| 1:A:8:MET:HE3 | 1:B:104:LEU:HD23 | 0.59 | 1.75 | 7 | 1 |
| 1:A:6:ILE:HD13 | 1:B:135:LEU:HD11 | 0.59 | 1.74 | 5 | 1 |
| 1:B:113:HIS:CD2 | 1:B:117:LYS:HG2 | 0.59 | 2.32 | 12 | 1 |
| 1:B:104:LEU:HD11 | 1:B:106:ILE:HG12 | 0.58 | 1.75 | 18 | 6 |
| 1:B:116:LEU:HD22 | 1:B:116:LEU:O | 0.58 | 1.99 | 8 | 1 |
| 1:A:35:LEU:HD21 | 1:B:135:LEU:HD21 | 0.58 | 1.74 | 11 | 5 |
| 1:A:16:LEU:HD23 | 1:A:27:ILE:HD12 | 0.58 | 1.75 | 21 | 2 |
| 1:B:132:LEU:O | 1:B:135:LEU:HD22 | 0.58 | 1.98 | 8 | 1 |
| 1:A:6:ILE:CG1 | 1:B:106:ILE:HD11 | 0.58 | 2.27 | 3 | 1 |
| 1:A:31:ALA:O | 1:A:35:LEU:HD22 | 0.58 | 1.97 | 15 | 1 |
| 1:A:9:THR:HG23 | 1:A:12:GLN:HB2 | 0.58 | 1.75 | 1 | 5 |
| 1:A:6:ILE:HG22 | 1:A:8:MET:SD | 0.57 | 2.38 | 20 | 4 |
| 1:A:32:LEU:HD23 | 1:B:106:ILE:CG2 | 0.57 | 2.28 | 21 | 1 |
| 1:B:117:LYS:CD | 1:B:127:ILE:HD13 | 0.57 | 2.29 | 12 | 1 |
| 1:B:116:LEU:HD12 | 1:B:130:TYR:CD2 | 0.57 | 2.35 | 6 | 1 |
| 1:A:32:LEU:C | 1:A:32:LEU:HD13 | 0.57 | 2.20 | 9 | 4 |
| 1:A:27:ILE:O | 1:A:31:ALA:HB3 | 0.57 | 1.99 | 7 | 2 |
| 1:B:116:LEU:HD12 | 1:B:130:TYR:CE2 | 0.57 | 2.34 | 6 | 3 |
| 1:A:4:LEU:HD11 | 1:A:6:ILE:HD11 | 0.57 | 1.76 | 23 | 1 |
| 1:B:106:ILE:HD13 | 1:B:108:MET:CE | 0.57 | 2.30 | 4 | 2 |
| 1:A:19:LEU:HA | 1:A:22:LEU:HD22 | 0.57 | 1.77 | 22 | 1 |
| 1:A:27:ILE:HG12 | 1:A:31:ALA:HB2 | 0.56 | 1.77 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:120:ALA:CB | 1:B:127:ILE:HA | 0.56 | 2.30 | 5 | 20 |
| 1:B:116:LEU:HD23 | 1:B:117:LYS:NZ | 0.56 | 2.15 | 5 | 1 |
| 1:A:13:HIS:HA | 1:A:16:LEU:HD11 | 0.56 | 1.77 | 15 | 2 |
| 1:A:32:LEU:HD11 | 1:B:112:GLN:OE1 | 0.56 | 1.99 | 24 | 1 |
| 1:A:20:ALA:HB1 | 1:A:27:ILE:N | 0.56 | 2.15 | 19 | 16 |
| 1:A:19:LEU:HD22 | 1:A:30:TYR:OH | 0.56 | 2.00 | 8 | 2 |
| 1:A:19:LEU:HD21 | 1:A:30:TYR:CZ | 0.56 | 2.35 | 4 | 1 |
| 1:B:113:HIS:HA | 1:B:117:LYS:CE | 0.56 | 2.30 | 12 | 1 |
| 1:B:117:LYS:HD2 | 1:B:127:ILE:CG1 | 0.56 | 2.30 | 12 | 1 |
| 1:A:19:LEU:HD11 | 1:A:30:TYR:OH | 0.56 | 2.01 | 13 | 1 |
| 1:A:35:LEU:HD23 | 1:B:131:ALA:HB1 | 0.56 | 1.76 | 14 | 1 |
| 1:A:32:LEU:C | 1:A:32:LEU:HD23 | 0.56 | 2.21 | 1 | 4 |
| 1:B:120:ALA:HB2 | 1:B:127:ILE:HA | 0.56 | 1.76 | 8 | 5 |
| 1:A:35:LEU:CD2 | 1:B:135:LEU:HD21 | 0.56 | 2.31 | 23 | 3 |
| 1:B:116:LEU:HD11 | 1:B:127:ILE:CG1 | 0.55 | 2.31 | 15 | 1 |
| 1:A:16:LEU:HD23 | 1:A:17:LYS:H | 0.55 | 1.60 | 14 | 1 |
| 1:A:49:LEU:HD11 | 1:A:50:LYS:HD3 | 0.55 | 1.78 | 24 | 1 |
| 1:B:113:HIS:HA | 1:B:117:LYS:HD3 | 0.55 | 1.78 | 5 | 1 |
| 1:A:13:HIS:O | 1:A:17:LYS:CG | 0.55 | 2.55 | 19 | 1 |
| 1:B:116:LEU:HD21 | 1:B:131:ALA:HB2 | 0.55 | 1.79 | 8 | 2 |
| 1:A:17:LYS:HD2 | 1:A:27:ILE:CG1 | 0.55 | 2.32 | 19 | 2 |
| 1:A:27:ILE:HG13 | 1:A:31:ALA:CB | 0.55 | 2.32 | 12 | 7 |
| 1:B:106:ILE:HG22 | 1:B:108:MET:SD | 0.55 | 2.42 | 12 | 3 |
| 1:A:16:LEU:HD12 | 1:B:135:LEU:HD23 | 0.55 | 1.77 | 17 | 1 |
| 1:A:17:LYS:N | 1:A:17:LYS:CD | 0.55 | 2.63 | 13 | 2 |
| 1:B:117:LYS:N | 1:B:117:LYS:CD | 0.55 | 2.66 | 12 | 1 |
| 1:A:31:ALA:HA | 1:B:135:LEU:HD22 | 0.55 | 1.79 | 14 | 2 |
| 1:A:6:ILE:HG23 | 1:A:8:MET:SD | 0.54 | 2.43 | 18 | 1 |
| 1:A:35:LEU:HD22 | 1:B:131:ALA:CB | 0.54 | 2.32 | 2 | 5 |
| 1:A:49:LEU:HD11 | 1:A:50:LYS:CD | 0.54 | 2.32 | 24 | 1 |
| 1:A:14:GLN:O | 1:A:18:ALA:CB | 0.54 | 2.56 | 4 | 8 |
| 1:A:35:LEU:HG | 1:B:131:ALA:HB1 | 0.54 | 1.79 | 15 | 1 |
| 1:A:17:LYS:HZ3 | 1:B:104:LEU:HD22 | 0.54 | 1.62 | 13 | 1 |
| 1:A:5:THR:O | 1:A:6:ILE:HD13 | 0.54 | 2.03 | 3 | 1 |
| 1:A:31:ALA:HB1 | 1:B:135:LEU:HD11 | 0.54 | 1.78 | 17 | 1 |
| 1:B:119:LEU:HD22 | 1:B:130:TYR:OH | 0.54 | 2.03 | 15 | 4 |
| 1:A:35:LEU:HD23 | 1:B:131:ALA:O | 0.54 | 2.03 | 8 | 2 |
| 1:A:35:LEU:HB3 | 1:B:116:LEU:HD22 | 0.54 | 1.79 | 18 | 1 |
| 1:A:6:ILE:O | 1:B:104:LEU:N | 0.53 | 2.41 | 18 | 7 |
| 1:A:4:LEU:HD23 | 1:A:6:ILE:HD11 | 0.53 | 1.80 | 10 | 2 |
| 1:A:4:LEU:HD21 | 1:A:6:ILE:CD1 | 0.53 | 2.23 | 11 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:32:LEU:HD21 | 1:B:112:GLN:OE1 | 0.53 | 2.03 | 7 | 1 |
| 1:A:35:LEU:HD12 | 1:B:108:MET:HE1 | 0.53 | 1.79 | 16 | 5 |
| 1:B:127:ILE:HD12 | 1:B:127:ILE:O | 0.53 | 2.03 | 24 | 2 |
| 1:A:4:LEU:HD12 | 1:A:5:THR:N | 0.53 | 2.18 | 7 | 2 |
| 1:A:53:LEU:HD22 | 1:A:53:LEU:H | 0.53 | 1.63 | 8 | 1 |
| 1:B:116:LEU:HD21 | 1:B:127:ILE:HD11 | 0.53 | 1.78 | 15 | 1 |
| 1:A:35:LEU:HD12 | 1:B:108:MET:HE3 | 0.53 | 1.80 | 23 | 1 |
| 1:B:127:ILE:HG13 | 1:B:131:ALA:CB | 0.53 | 2.33 | 22 | 6 |
| 1:A:16:LEU:HD22 | 1:B:135:LEU:CB | 0.53 | 2.34 | 12 | 2 |
| 1:A:32:LEU:HD13 | 1:A:33:GLU:N | 0.53 | 2.19 | 7 | 3 |
| 1:A:31:ALA:O | 1:A:35:LEU:CD2 | 0.53 | 2.57 | 15 | 1 |
| 1:B:131:ALA:O | 1:B:135:LEU:HG | 0.53 | 2.03 | 10 | 7 |
| 1:A:16:LEU:HD13 | 1:A:30:TYR:HE2 | 0.53 | 1.59 | 19 | 4 |
| 1:B:113:HIS:HA | 1:B:117:LYS:HE3 | 0.53 | 1.81 | 12 | 1 |
| 1:B:132:LEU:O | 1:B:132:LEU:HD12 | 0.53 | 2.04 | 20 | 1 |
| 1:A:32:LEU:HD13 | 1:A:32:LEU:C | 0.53 | 2.24 | 7 | 1 |
| 1:A:19:LEU:HA | 1:A:22:LEU:CD2 | 0.53 | 2.32 | 15 | 2 |
| 1:A:9:THR:HG22 | 1:A:12:GLN:CG | 0.53 | 2.34 | 22 | 1 |
| 1:B:116:LEU:HD23 | 1:B:117:LYS:HZ1 | 0.53 | 1.63 | 5 | 1 |
| 1:A:28:LYS:O | 1:B:106:ILE:HD11 | 0.53 | 2.04 | 16 | 3 |
| 1:A:8:MET:CE | 1:B:132:LEU:HD12 | 0.53 | 2.34 | 17 | 1 |
| 1:A:35:LEU:O | 1:B:116:LEU:HD13 | 0.53 | 2.04 | 18 | 1 |
| 1:A:6:ILE:HD13 | 1:A:6:ILE:N | 0.53 | 2.18 | 24 | 1 |
| 1:A:13:HIS:HA | 1:A:17:LYS:HE3 | 0.53 | 1.81 | 13 | 1 |
| 1:A:12:GLN:OE1 | 1:B:132:LEU:HD21 | 0.53 | 2.04 | 16 | 1 |
| 1:A:51:THR:O | 1:A:52:MET:CB | 0.52 | 2.57 | 22 | 1 |
| 1:A:6:ILE:HD11 | 1:B:106:ILE:HG12 | 0.52 | 1.82 | 3 | 1 |
| 1:A:35:LEU:HD22 | 1:B:131:ALA:CA | 0.52 | 2.35 | 12 | 4 |
| 1:A:16:LEU:HD12 | 1:A:27:ILE:HD12 | 0.52 | 1.81 | 10 | 1 |
| 1:A:17:LYS:HD2 | 1:A:27:ILE:HD13 | 0.52 | 1.82 | 19 | 2 |
| 1:B:113:HIS:HA | 1:B:116:LEU:HD23 | 0.52 | 1.81 | 14 | 2 |
| 1:A:35:LEU:HD12 | 1:B:131:ALA:O | 0.52 | 2.03 | 15 | 1 |
| 1:A:20:ALA:HB1 | 1:A:27:ILE:CA | 0.52 | 2.34 | 23 | 4 |
| 1:A:35:LEU:CG | 1:B:135:LEU:HD21 | 0.52 | 2.33 | 21 | 2 |
| 1:B:104:LEU:HD21 | 1:B:106:ILE:CD1 | 0.52 | 2.34 | 10 | 1 |
| 1:B:106:ILE:CG2 | 1:B:108:MET:HE2 | 0.52 | 2.34 | 19 | 2 |
| 1:A:6:ILE:HG13 | 1:B:106:ILE:HD11 | 0.52 | 1.81 | 3 | 1 |
| 1:A:32:LEU:HG | 1:B:106:ILE:HD11 | 0.52 | 1.81 | 22 | 1 |
| 1:B:116:LEU:HD11 | 1:B:127:ILE:HD12 | 0.52 | 1.79 | 2 | 1 |
| 1:A:28:LYS:HA | 1:B:106:ILE:HG13 | 0.52 | 1.81 | 13 | 4 |
| 1:B:132:LEU:C | 1:B:132:LEU:HD13 | 0.51 | 2.25 | 16 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:53:LEU:H | 1:A:53:LEU:HD22 | 0.51 | 1.63 | 7 | 1 |
| 1:B:127:ILE:HG12 | 1:B:131:ALA:CB | 0.51 | 2.36 | 11 | 1 |
| 1:B:132:LEU:HD23 | 1:B:132:LEU:C | 0.51 | 2.26 | 23 | 2 |
| 1:B:109:THR:HG22 | 1:B:112:GLN:CG | 0.51 | 2.35 | 24 | 1 |
| 1:B:127:ILE:HG13 | 1:B:131:ALA:HB3 | 0.51 | 1.82 | 4 | 1 |
| 1:A:16:LEU:HD12 | 1:A:27:ILE:CD1 | 0.51 | 2.36 | 10 | 1 |
| 1:A:30:TYR:CE1 | 1:A:34:ARG:NE | 0.51 | 2.79 | 7 | 1 |
| 1:A:5:THR:HG21 | 1:B:103:ARG:CZ | 0.51 | 2.36 | 18 | 1 |
| 1:B:117:LYS:HE3 | 1:B:127:ILE:HD13 | 0.51 | 1.83 | 10 | 1 |
| 1:B:117:LYS:CG | 1:B:127:ILE:HG21 | 0.50 | 2.34 | 24 | 2 |
| 1:A:35:LEU:N | 1:A:35:LEU:CD1 | 0.50 | 2.75 | 15 | 1 |
| 1:B:113:HIS:HA | 1:B:116:LEU:HD11 | 0.50 | 1.82 | 23 | 1 |
| 1:B:113:HIS:CA | 1:B:117:LYS:HE3 | 0.50 | 2.37 | 12 | 1 |
| 1:A:4:LEU:HD13 | 1:B:127:ILE:CD1 | 0.50 | 2.37 | 16 | 1 |
| 1:B:106:ILE:HG23 | 1:B:108:MET:SD | 0.50 | 2.47 | 17 | 2 |
| 1:B:114:GLN:O | 1:B:118:ALA:HB2 | 0.50 | 2.07 | 12 | 2 |
| 1:A:16:LEU:HD11 | 1:B:135:LEU:O | 0.50 | 2.07 | 19 | 2 |
| 1:A:34:ARG:HB3 | 1:B:135:LEU:HD23 | 0.50 | 1.83 | 19 | 5 |
| 1:B:116:LEU:CD2 | 1:B:127:ILE:HD12 | 0.50 | 2.37 | 18 | 3 |
| 1:B:121:ALA:HA | 1:B:125:LYS:O | 0.50 | 2.07 | 4 | 11 |
| 1:B:120:ALA:CB | 1:B:127:ILE:CA | 0.50 | 2.90 | 24 | 13 |
| 1:B:130:TYR:CD1 | 1:B:131:ALA:N | 0.49 | 2.80 | 13 | 2 |
| 1:B:112:GLN:HG3 | 1:B:113:HIS:N | 0.49 | 2.22 | 20 | 4 |
| 1:A:35:LEU:CD2 | 1:B:135:LEU:HD11 | 0.49 | 2.37 | 8 | 1 |
| 1:A:12:GLN:HG3 | 1:A:13:HIS:N | 0.49 | 2.22 | 22 | 2 |
| 1:A:46:TRP:HB3 | 1:A:49:LEU:HD23 | 0.49 | 1.84 | 5 | 1 |
| 1:A:5:THR:HG22 | 1:B:103:ARG:HD2 | 0.49 | 1.84 | 6 | 1 |
| 1:A:8:MET:HE3 | 1:B:135:LEU:HD12 | 0.49 | 1.85 | 9 | 1 |
| 1:A:13:HIS:CG | 1:B:102:SER:HB3 | 0.49 | 2.42 | 23 | 1 |
| 1:A:53:LEU:H | 1:A:53:LEU:CD1 | 0.49 | 2.16 | 7 | 2 |
| 1:B:113:HIS:O | 1:B:116:LEU:HD13 | 0.49 | 2.08 | 7 | 2 |
| 1:A:31:ALA:O | 1:A:35:LEU:HD12 | 0.49 | 2.08 | 14 | 2 |
| 1:A:13:HIS:CD2 | 1:A:17:LYS:HB2 | 0.49 | 2.41 | 23 | 1 |
| 1:B:109:THR:HG22 | 1:B:112:GLN:HG2 | 0.49 | 1.85 | 24 | 1 |
| 1:A:49:LEU:C | 1:A:49:LEU:HD12 | 0.49 | 2.28 | 24 | 2 |
| 1:A:14:GLN:O | 1:A:18:ALA:HB2 | 0.49 | 2.08 | 13 | 2 |
| 1:A:53:LEU:N | 1:A:53:LEU:HD13 | 0.49 | 2.22 | 8 | 1 |
| 1:B:116:LEU:HD23 | 1:B:127:ILE:HD13 | 0.49 | 1.84 | 23 | 1 |
| 1:B:113:HIS:HA | 1:B:117:LYS:CD | 0.49 | 2.38 | 5 | 1 |
| 1:A:32:LEU:CA | 1:B:106:ILE:HD11 | 0.49 | 2.37 | 22 | 1 |
| 1:A:28:LYS:HD2 | 1:B:106:ILE:HG23 | 0.49 | 1.85 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:127:ILE:CD1 | 1:B:131:ALA:CB | 0.49 | 2.89 | 24 | 2 |
| 1:B:108:MET:HB3 | 1:B:112:GLN:NE2 | 0.49 | 2.23 | 24 | 2 |
| 1:B:127:ILE:HD12 | 1:B:131:ALA:CB | 0.48 | 2.37 | 24 | 2 |
| 1:A:16:LEU:HD22 | 1:A:19:LEU:CD2 | 0.48 | 2.38 | 13 | 1 |
| 1:A:16:LEU:HD11 | 1:A:27:ILE:HD11 | 0.48 | 1.84 | 8 | 4 |
| 1:A:35:LEU:HB3 | 1:B:116:LEU:HD13 | 0.48 | 1.84 | 5 | 1 |
| 1:B:116:LEU:HD13 | 1:B:127:ILE:HD13 | 0.48 | 1.86 | 13 | 2 |
| 1:B:104:LEU:HD11 | 1:B:106:ILE:HD11 | 0.48 | 1.85 | 19 | 1 |
| 1:A:35:LEU:CD2 | 1:B:135:LEU:HG | 0.48 | 2.39 | 11 | 1 |
| 1:A:13:HIS:CG | 1:B:102:SER:CB | 0.48 | 2.96 | 23 | 1 |
| 1:A:28:LYS:HE3 | 1:B:105:THR:O | 0.48 | 2.07 | 6 | 2 |
| 1:A:3:ARG:CD | 1:B:105:THR:HG22 | 0.48 | 2.39 | 17 | 2 |
| 1:A:30:TYR:CD1 | 1:A:31:ALA:N | 0.48 | 2.82 | 15 | 1 |
| 1:A:8:MET:HB2 | 1:B:102:SER:N | 0.48 | 2.24 | 23 | 1 |
| 1:A:16:LEU:HD21 | 1:A:27:ILE:HD11 | 0.48 | 1.86 | 3 | 1 |
| 1:B:106:ILE:HG21 | 1:B:108:MET:CE | 0.48 | 2.38 | 23 | 4 |
| 1:A:27:ILE:HG13 | 1:A:31:ALA:HB3 | 0.48 | 1.85 | 2 | 1 |
| 1:A:35:LEU:CD1 | 1:B:131:ALA:HB1 | 0.48 | 2.39 | 10 | 1 |
| 1:A:13:HIS:O | 1:A:17:LYS:HG2 | 0.48 | 2.07 | 19 | 2 |
| 1:A:4:LEU:HD11 | 1:A:6:ILE:HG13 | 0.48 | 1.85 | 19 | 2 |
| 1:A:13:HIS:CD2 | 1:A:17:LYS:CE | 0.48 | 2.96 | 19 | 1 |
| 1:B:106:ILE:CG2 | 1:B:108:MET:SD | 0.47 | 3.02 | 12 | 4 |
| 1:B:113:HIS:CA | 1:B:117:LYS:HD3 | 0.47 | 2.39 | 5 | 1 |
| 1:A:53:LEU:H | 1:A:53:LEU:CD2 | 0.47 | 2.22 | 7 | 1 |
| 1:A:16:LEU:HD11 | 1:A:27:ILE:HD12 | 0.47 | 1.86 | 8 | 2 |
| 1:A:8:MET:HE2 | 1:B:132:LEU:HD12 | 0.47 | 1.86 | 17 | 1 |
| 1:B:116:LEU:CG | 1:B:127:ILE:HD12 | 0.47 | 2.39 | 15 | 1 |
| 1:A:6:ILE:CG2 | 1:A:8:MET:SD | 0.47 | 3.03 | 9 | 5 |
| 1:B:116:LEU:HD12 | 1:B:116:LEU:C | 0.47 | 2.29 | 15 | 2 |
| 1:A:4:LEU:HD11 | 1:A:6:ILE:CD1 | 0.47 | 2.40 | 23 | 1 |
| 1:A:4:LEU:HD22 | 1:B:127:ILE:CD1 | 0.47 | 2.40 | 18 | 6 |
| 1:A:40:ALA:HB2 | 1:B:134:ARG:CZ | 0.47 | 2.39 | 16 | 1 |
| 1:A:53:LEU:HD13 | 1:A:53:LEU:N | 0.47 | 2.22 | 7 | 1 |
| 1:A:13:HIS:HA | 1:A:16:LEU:HD21 | 0.47 | 1.85 | 10 | 1 |
| 1:A:27:ILE:O | 1:A:31:ALA:N | 0.47 | 2.41 | 13 | 3 |
| 1:A:4:LEU:HD23 | 1:B:108:MET:SD | 0.47 | 2.49 | 23 | 2 |
| 1:A:4:LEU:CD2 | 1:A:35:LEU:CD1 | 0.47 | 2.93 | 16 | 1 |
| 1:A:6:ILE:HD11 | 1:B:132:LEU:CB | 0.47 | 2.36 | 16 | 1 |
| 1:A:8:MET:HG3 | 1:B:102:SER:O | 0.47 | 2.09 | 23 | 1 |
| 1:A:8:MET:CG | 1:B:102:SER:O | 0.47 | 2.63 | 23 | 1 |
| 1:A:32:LEU:HD12 | 1:B:107:ASP:O | 0.47 | 2.09 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:28:LYS:CD | 1:B:106:ILE:HG23 | 0.47 | 2.39 | 2 | 1 |
| 1:A:35:LEU:HD21 | 1:B:135:LEU:CG | 0.47 | 2.39 | 6 | 2 |
| 1:A:20:ALA:O | 1:A:25:LYS:O | 0.47 | 2.33 | 22 | 1 |
| 1:A:32:LEU:HD23 | 1:A:32:LEU:O | 0.47 | 2.10 | 5 | 4 |
| 1:A:35:LEU:CB | 1:B:116:LEU:HD22 | 0.47 | 2.40 | 15 | 1 |
| 1:A:16:LEU:HD12 | 1:A:30:TYR:CD2 | 0.46 | 2.44 | 12 | 2 |
| 1:A:5:THR:O | 1:B:128:LYS:CE | 0.46 | 2.62 | 17 | 3 |
| 1:B:116:LEU:C | 1:B:116:LEU:CD2 | 0.46 | 2.84 | 7 | 3 |
| 1:A:35:LEU:HB2 | 1:B:116:LEU:HD11 | 0.46 | 1.86 | 10 | 1 |
| 1:A:5:THR:HG22 | 1:B:103:ARG:CD | 0.46 | 2.41 | 6 | 1 |
| 1:B:109:THR:HG23 | 1:B:112:GLN:CB | 0.46 | 2.41 | 15 | 1 |
| 1:B:117:LYS:HD2 | 1:B:117:LYS:H | 0.46 | 1.70 | 5 | 1 |
| 1:A:4:LEU:HD13 | 1:B:127:ILE:HD13 | 0.46 | 1.86 | 6 | 3 |
| 1:A:35:LEU:HD22 | 1:B:131:ALA:O | 0.46 | 2.10 | 17 | 1 |
| 1:A:6:ILE:CG2 | 1:A:8:MET:CE | 0.46 | 2.94 | 18 | 3 |
| 1:A:16:LEU:HD21 | 1:A:27:ILE:CG1 | 0.46 | 2.40 | 7 | 3 |
| 1:A:16:LEU:C | 1:A:16:LEU:CD2 | 0.46 | 2.84 | 20 | 4 |
| 1:A:13:HIS:O | 1:A:16:LEU:HD13 | 0.46 | 2.10 | 7 | 2 |
| 1:A:21:ALA:HA | 1:A:25:LYS:O | 0.46 | 2.11 | 12 | 7 |
| 1:A:27:ILE:HD11 | 1:B:104:LEU:CD2 | 0.46 | 2.40 | 2 | 1 |
| 1:A:48:GLU:HA | 1:A:52:MET:CA | 0.46 | 2.41 | 22 | 1 |
| 1:A:31:ALA:O | 1:B:135:LEU:CD2 | 0.46 | 2.63 | 2 | 5 |
| 1:A:17:LYS:HZ2 | 1:B:104:LEU:HD22 | 0.46 | 1.66 | 13 | 1 |
| 1:A:17:LYS:CE | 1:A:17:LYS:O | 0.46 | 2.64 | 5 | 4 |
| 1:A:19:LEU:O | 1:A:22:LEU:CD2 | 0.46 | 2.56 | 22 | 1 |
| 1:B:130:TYR:CE1 | 1:B:134:ARG:NH1 | 0.46 | 2.84 | 23 | 1 |
| 1:A:4:LEU:CD2 | 1:B:127:ILE:HD11 | 0.46 | 2.40 | 13 | 2 |
| 1:A:7:ASP:O | 1:B:132:LEU:HD11 | 0.46 | 2.11 | 8 | 1 |
| 1:A:32:LEU:HA | 1:A:35:LEU:CD2 | 0.46 | 2.41 | 15 | 1 |
| 1:A:41:ASP:O | 1:A:45:ALA:HB3 | 0.46 | 2.10 | 15 | 1 |
| 1:A:6:ILE:HG21 | 1:A:8:MET:CE | 0.45 | 2.41 | 6 | 1 |
| 1:B:117:LYS:HD2 | 1:B:127:ILE:HD13 | 0.45 | 1.87 | 12 | 1 |
| 1:A:17:LYS:HD2 | 1:A:27:ILE:CD1 | 0.45 | 2.41 | 19 | 2 |
| 1:A:17:LYS:CG | 1:A:27:ILE:HG21 | 0.45 | 2.36 | 15 | 1 |
| 1:B:104:LEU:HG | 1:B:104:LEU:O | 0.45 | 2.11 | 23 | 1 |
| 1:A:13:HIS:CE1 | 1:B:104:LEU:CB | 0.45 | 2.99 | 1 | 4 |
| 1:A:6:ILE:HG21 | 1:A:8:MET:HE3 | 0.45 | 1.88 | 7 | 1 |
| 1:B:113:HIS:O | 1:B:117:LYS:HG2 | 0.45 | 2.12 | 12 | 1 |
| 1:A:20:ALA:CB | 1:A:27:ILE:N | 0.45 | 2.79 | 1 | 5 |
| 1:B:120:ALA:CB | 1:B:127:ILE:N | 0.45 | 2.80 | 6 | 9 |
| 1:B:114:GLN:O | 1:B:118:ALA:HB3 | 0.45 | 2.12 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:135:LEU:N | 1:B:135:LEU:CD1 | 0.45 | 2.79 | 8 | 1 |
| 1:A:53:LEU:HD12 | 1:A:53:LEU:C | 0.45 | 2.32 | 5 | 1 |
| 1:A:4:LEU:CD2 | 1:A:6:ILE:CD1 | 0.45 | 2.95 | 3 | 1 |
| 1:A:31:ALA:CA | 1:B:135:LEU:HD22 | 0.45 | 2.42 | 9 | 5 |
| 1:B:114:GLN:O | 1:B:118:ALA:CB | 0.45 | 2.64 | 18 | 3 |
| 1:A:16:LEU:HG | 1:A:17:LYS:N | 0.45 | 2.26 | 18 | 2 |
| 1:B:132:LEU:HD23 | 1:B:132:LEU:O | 0.45 | 2.12 | 23 | 2 |
| 1:B:130:TYR:CE1 | 1:B:134:ARG:CZ | 0.45 | 3.00 | 23 | 1 |
| 1:A:20:ALA:HB2 | 1:A:27:ILE:HA | 0.45 | 1.87 | 1 | 3 |
| 1:A:2:SER:O | 1:B:108:MET:N | 0.45 | 2.49 | 17 | 2 |
| 1:A:35:LEU:HB3 | 1:B:116:LEU:HD11 | 0.45 | 1.89 | 10 | 1 |
| 1:A:9:THR:CG2 | 1:A:12:GLN:CB | 0.45 | 2.95 | 21 | 1 |
| 1:A:2:SER:CB | 1:B:108:MET:O | 0.45 | 2.65 | 18 | 3 |
| 1:B:127:ILE:CG1 | 1:B:131:ALA:CB | 0.45 | 2.95 | 6 | 2 |
| 1:A:16:LEU:HD12 | 1:A:17:LYS:H | 0.45 | 1.71 | 24 | 1 |
| 1:A:13:HIS:O | 1:A:17:LYS:HB3 | 0.45 | 2.11 | 18 | 1 |
| 1:A:6:ILE:HD11 | 1:B:128:LYS:O | 0.44 | 2.12 | 7 | 1 |
| 1:A:13:HIS:O | 1:A:17:LYS:HE3 | 0.44 | 2.12 | 13 | 1 |
| 1:A:8:MET:O | 1:B:102:SER:CB | 0.44 | 2.65 | 4 | 2 |
| 1:A:27:ILE:HD13 | 1:B:104:LEU:HD22 | 0.44 | 1.87 | 9 | 1 |
| 1:A:35:LEU:HB2 | 1:B:116:LEU:HD22 | 0.44 | 1.89 | 15 | 1 |
| 1:A:4:LEU:N | 1:B:106:ILE:O | 0.44 | 2.51 | 23 | 8 |
| 1:A:46:TRP:CB | 1:A:49:LEU:HD23 | 0.44 | 2.43 | 5 | 1 |
| 1:A:35:LEU:CD2 | 1:B:135:LEU:CD2 | 0.44 | 2.96 | 6 | 2 |
| 1:A:35:LEU:CD1 | 1:B:135:LEU:HD21 | 0.44 | 2.41 | 13 | 1 |
| 1:A:16:LEU:CD1 | 1:A:17:LYS:N | 0.44 | 2.81 | 24 | 1 |
| 1:A:32:LEU:HD13 | 1:A:32:LEU:O | 0.44 | 2.12 | 10 | 1 |
| 1:B:116:LEU:HD13 | 1:B:130:TYR:HE2 | 0.44 | 1.73 | 12 | 2 |
| 1:A:16:LEU:HD23 | 1:A:27:ILE:CD1 | 0.44 | 2.38 | 15 | 1 |
| 1:A:6:ILE:CG2 | 1:A:8:MET:HE3 | 0.44 | 2.42 | 7 | 1 |
| 1:B:116:LEU:HD12 | 1:B:117:LYS:H | 0.44 | 1.69 | 3 | 1 |
| 1:A:20:ALA:CB | 1:A:27:ILE:CA | 0.44 | 2.96 | 19 | 5 |
| 1:A:28:LYS:CE | 1:B:105:THR:O | 0.44 | 2.65 | 16 | 2 |
| 1:B:131:ALA:O | 1:B:135:LEU:N | 0.44 | 2.51 | 10 | 2 |
| 1:B:117:LYS:HE3 | 1:B:127:ILE:CG1 | 0.44 | 2.42 | 10 | 1 |
| 1:A:13:HIS:HA | 1:A:16:LEU:CD1 | 0.44 | 2.42 | 15 | 1 |
| 1:B:109:THR:CG2 | 1:B:112:GLN:CB | 0.44 | 2.96 | 15 | 1 |
| 1:A:27:ILE:HG23 | 1:A:28:LYS:HD3 | 0.43 | 1.89 | 4 | 1 |
| 1:A:16:LEU:CD1 | 1:A:27:ILE:CD1 | 0.43 | 2.95 | 10 | 2 |
| 1:A:16:LEU:HD12 | 1:A:17:LYS:N | 0.43 | 2.28 | 24 | 1 |
| 1:A:11:GLN:O | 1:A:14:GLN:CG | 0.43 | 2.66 | 17 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:106:ILE:HD13 | 1:B:108:MET:HE2 | 0.43 | 1.88 | 24 | 2 |
| 1:A:20:ALA:HB1 | 1:A:26:THR:C | 0.43 | 2.34 | 22 | 2 |
| 1:A:28:LYS:O | 1:A:32:LEU:HB2 | 0.43 | 2.13 | 1 | 1 |
| 1:A:13:HIS:CA | 1:A:17:LYS:HE3 | 0.43 | 2.43 | 13 | 1 |
| 1:B:117:LYS:O | 1:B:117:LYS:CE | 0.43 | 2.66 | 20 | 4 |
| 1:A:3:ARG:HD3 | 1:B:105:THR:HG22 | 0.43 | 1.89 | 20 | 1 |
| 1:A:8:MET:CB | 1:B:102:SER:O | 0.43 | 2.67 | 23 | 1 |
| 1:A:53:LEU:N | 1:A:53:LEU:CD2 | 0.43 | 2.77 | 8 | 1 |
| 1:B:130:TYR:OH | 1:B:134:ARG:CZ | 0.43 | 2.67 | 10 | 1 |
| 1:A:27:ILE:CG1 | 1:A:31:ALA:CB | 0.43 | 2.96 | 9 | 2 |
| 1:B:120:ALA:HB1 | 1:B:127:ILE:CA | 0.43 | 2.44 | 23 | 2 |
| 1:A:17:LYS:HA | 1:A:27:ILE:HB | 0.43 | 1.89 | 18 | 1 |
| 1:A:16:LEU:CD2 | 1:A:27:ILE:CD1 | 0.43 | 2.96 | 3 | 1 |
| 1:B:119:LEU:HB3 | 1:B:130:TYR:CE2 | 0.43 | 2.49 | 10 | 2 |
| 1:A:35:LEU:CD2 | 1:B:131:ALA:O | 0.43 | 2.67 | 2 | 4 |
| 1:B:106:ILE:CG2 | 1:B:108:MET:CE | 0.43 | 2.97 | 23 | 3 |
| 1:A:16:LEU:HG | 1:A:27:ILE:CD1 | 0.43 | 2.44 | 3 | 1 |
| 1:A:28:LYS:HD3 | 1:B:106:ILE:HG23 | 0.43 | 1.90 | 6 | 1 |
| 1:A:49:LEU:HD12 | 1:A:49:LEU:C | 0.43 | 2.32 | 8 | 1 |
| 1:B:116:LEU:HD13 | 1:B:130:TYR:CE2 | 0.43 | 2.48 | 12 | 2 |
| 1:A:13:HIS:O | 1:A:17:LYS:HE2 | 0.43 | 2.14 | 19 | 1 |
| 1:A:16:LEU:HD23 | 1:B:135:LEU:CB | 0.43 | 2.40 | 24 | 1 |
| 1:B:104:LEU:CD2 | 1:B:135:LEU:CD1 | 0.43 | 2.96 | 7 | 1 |
| 1:A:5:THR:O | 1:B:128:LYS:HE2 | 0.43 | 2.13 | 12 | 1 |
| 1:A:8:MET:HB3 | 1:A:12:GLN:NE2 | 0.43 | 2.29 | 16 | 1 |
| 1:B:109:THR:HG23 | 1:B:112:GLN:HB2 | 0.42 | 1.91 | 12 | 1 |
| 1:A:2:SER:O | 1:B:108:MET:CB | 0.42 | 2.67 | 17 | 1 |
| 1:A:16:LEU:CD2 | 1:A:31:ALA:HB2 | 0.42 | 2.43 | 21 | 1 |
| 1:B:116:LEU:H | 1:B:116:LEU:HD13 | 0.42 | 1.74 | 23 | 1 |
| 1:B:116:LEU:CD1 | 1:B:127:ILE:CD1 | 0.42 | 2.89 | 3 | 2 |
| 1:A:8:MET:CE | 1:B:135:LEU:HD23 | 0.42 | 2.43 | 8 | 1 |
| 1:B:113:HIS:O | 1:B:113:HIS:CD2 | 0.42 | 2.72 | 11 | 2 |
| 1:A:35:LEU:HG | 1:B:135:LEU:CD2 | 0.42 | 2.43 | 21 | 1 |
| 1:A:6:ILE:CG2 | 1:A:8:MET:HE2 | 0.42 | 2.44 | 2 | 2 |
| 1:B:116:LEU:HD23 | 1:B:117:LYS:CE | 0.42 | 2.45 | 5 | 1 |
| 1:B:120:ALA:HB1 | 1:B:127:ILE:HA | 0.42 | 1.90 | 23 | 2 |
| 1:A:7:ASP:O | 1:B:132:LEU:CD1 | 0.42 | 2.67 | 8 | 1 |
| 1:A:28:LYS:CD | 1:B:105:THR:O | 0.42 | 2.67 | 9 | 2 |
| 1:B:120:ALA:HA | 1:B:130:TYR:CG | 0.42 | 2.50 | 10 | 1 |
| 1:B:116:LEU:CD2 | 1:B:127:ILE:CD1 | 0.42 | 2.97 | 18 | 2 |
| 1:B:117:LYS:HD2 | 1:B:127:ILE:CD1 | 0.42 | 2.44 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:13:HIS:CE1 | 1:B:104:LEU:HB3 | 0.42 | 2.50 | 14 | 1 |
| 1:A:13:HIS:NE2 | 1:A:17:LYS:HG3 | 0.42 | 2.28 | 23 | 1 |
| 1:B:123:GLN:OE1 | 1:B:130:TYR:CD1 | 0.42 | 2.73 | 16 | 2 |
| 1:A:9:THR:OG1 | 1:A:12:GLN:HG2 | 0.42 | 2.14 | 20 | 1 |
| 1:B:113:HIS:O | 1:B:117:LYS:HD3 | 0.42 | 2.14 | 5 | 1 |
| 1:B:119:LEU:HB3 | 1:B:130:TYR:CZ | 0.42 | 2.49 | 10 | 1 |
| 1:B:109:THR:CG2 | 1:B:112:GLN:CG | 0.42 | 2.97 | 13 | 1 |
| 1:A:6:ILE:HG12 | 1:B:106:ILE:HD11 | 0.42 | 1.92 | 3 | 1 |
| 1:A:13:HIS:ND1 | 1:B:102:SER:CB | 0.42 | 2.82 | 23 | 1 |
| 1:A:27:ILE:CD1 | 1:B:104:LEU:HD13 | 0.42 | 2.44 | 7 | 1 |
| 1:A:32:LEU:HD22 | 1:A:32:LEU:O | 0.42 | 2.14 | 7 | 1 |
| 1:B:120:ALA:O | 1:B:125:LYS:O | 0.42 | 2.38 | 10 | 1 |
| 1:A:4:LEU:HB2 | 1:B:113:HIS:CE1 | 0.42 | 2.50 | 19 | 1 |
| 1:A:16:LEU:O | 1:A:16:LEU:HD12 | 0.42 | 2.14 | 23 | 1 |
| 1:B:120:ALA:HB1 | 1:B:126:THR:C | 0.42 | 2.35 | 6 | 2 |
| 1:A:30:TYR:CE1 | 1:A:34:ARG:HD2 | 0.42 | 2.49 | 10 | 1 |
| 1:A:13:HIS:CD2 | 1:A:17:LYS:HE3 | 0.42 | 2.50 | 13 | 1 |
| 1:A:13:HIS:O | 1:A:13:HIS:CD2 | 0.42 | 2.73 | 20 | 4 |
| 1:A:16:LEU:HD13 | 1:A:27:ILE:HD13 | 0.42 | 1.91 | 24 | 1 |
| 1:A:23:GLN:OE1 | 1:A:30:TYR:CE1 | 0.42 | 2.73 | 1 | 1 |
| 1:A:27:ILE:HD12 | 1:A:27:ILE:O | 0.42 | 2.15 | 15 | 1 |
| 1:B:123:GLN:OE1 | 1:B:130:TYR:CG | 0.42 | 2.73 | 7 | 1 |
| 1:B:128:LYS:O | 1:B:132:LEU:HB2 | 0.42 | 2.14 | 8 | 1 |
| 1:A:5:THR:HG21 | 1:B:103:ARG:NE | 0.42 | 2.30 | 18 | 1 |
| 1:A:28:LYS:N | 1:A:28:LYS:CD | 0.41 | 2.83 | 4 | 1 |
| 1:B:117:LYS:HG3 | 1:B:127:ILE:HG21 | 0.41 | 1.91 | 10 | 1 |
| 1:B:117:LYS:HD2 | 1:B:127:ILE:CB | 0.41 | 2.45 | 12 | 1 |
| 1:A:27:ILE:HG12 | 1:A:31:ALA:CB | 0.41 | 2.44 | 1 | 1 |
| 1:A:4:LEU:CB | 1:B:113:HIS:CE1 | 0.41 | 3.03 | 11 | 1 |
| 1:A:16:LEU:HD13 | 1:A:16:LEU:C | 0.41 | 2.34 | 11 | 1 |
| 1:A:16:LEU:HA | 1:A:19:LEU:CD2 | 0.41 | 2.43 | 14 | 1 |
| 1:A:13:HIS:CA | 1:A:17:LYS:HE2 | 0.41 | 2.44 | 19 | 1 |
| 1:A:3:ARG:CG | 1:B:106:ILE:O | 0.41 | 2.69 | 16 | 1 |
| 1:A:5:THR:O | 1:B:128:LYS:CD | 0.41 | 2.69 | 20 | 1 |
| 1:B:104:LEU:CD1 | 1:B:106:ILE:CG1 | 0.41 | 2.97 | 23 | 1 |
| 1:B:106:ILE:N | 1:B:106:ILE:CD1 | 0.41 | 2.79 | 3 | 1 |
| 1:A:35:LEU:HD21 | 1:B:135:LEU:HD11 | 0.41 | 1.92 | 8 | 1 |
| 1:A:17:LYS:HD2 | 1:A:27:ILE:CB | 0.41 | 2.46 | 13 | 1 |
| 1:A:6:ILE:HD13 | 1:A:35:LEU:HD21 | 0.41 | 1.92 | 14 | 1 |
| 1:A:16:LEU:CD2 | 1:A:16:LEU:C | 0.41 | 2.88 | 15 | 1 |
| 1:A:46:TRP:CE3 | 1:A:49:LEU:CD1 | 0.41 | 3.04 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:35:LEU:HD13 | 1:B:116:LEU:CD2 | 0.41 | 2.46 | 5 | 1 |
| 1:B:106:ILE:HG21 | 1:B:108:MET:HE1 | 0.41 | 1.93 | 17 | 1 |
| 1:A:13:HIS:HA | 1:A:17:LYS:CE | 0.41 | 2.45 | 13 | 1 |
| 1:B:117:LYS:CE | 1:B:117:LYS:O | 0.41 | 2.69 | 1 | 1 |
| 1:A:35:LEU:HD21 | 1:B:131:ALA:O | 0.41 | 2.16 | 12 | 2 |
| 1:A:19:LEU:HB3 | 1:A:30:TYR:CE2 | 0.41 | 2.51 | 12 | 1 |
| 1:B:113:HIS:O | 1:B:117:LYS:CG | 0.41 | 2.69 | 12 | 1 |
| 1:A:17:LYS:O | 1:A:17:LYS:CE | 0.41 | 2.69 | 14 | 1 |
| 1:A:28:LYS:O | 1:A:32:LEU:CB | 0.41 | 2.69 | 18 | 1 |
| 1:B:117:LYS:HE3 | 1:B:127:ILE:HG22 | 0.41 | 1.93 | 22 | 1 |
| 1:A:16:LEU:HD13 | 1:A:27:ILE:CD1 | 0.41 | 2.46 | 24 | 1 |
| 1:B:111:GLN:O | 1:B:114:GLN:CG | 0.41 | 2.69 | 2 | 2 |
| 1:B:123:GLN:CG | 1:B:125:LYS:CG | 0.41 | 2.99 | 4 | 1 |
| 1:B:123:GLN:NE2 | 1:B:130:TYR:CD1 | 0.41 | 2.89 | 9 | 1 |
| 1:B:104:LEU:O | 1:B:104:LEU:HG | 0.41 | 2.16 | 20 | 1 |
| 1:A:41:ASP:OD1 | 1:A:45:ALA:HB2 | 0.41 | 2.16 | 21 | 1 |
| 1:B:128:LYS:CD | 1:B:128:LYS:N | 0.40 | 2.83 | 17 | 1 |
| 1:A:13:HIS:CE1 | 1:A:17:LYS:HG3 | 0.40 | 2.51 | 23 | 1 |
| 1:A:4:LEU:HB3 | 1:B:113:HIS:CE1 | 0.40 | 2.51 | 11 | 1 |
| 1:B:113:HIS:HA | 1:B:116:LEU:CD1 | 0.40 | 2.47 | 23 | 2 |
| 1:A:31:ALA:O | 1:A:35:LEU:CG | 0.40 | 2.69 | 14 | 1 |
| 1:B:117:LYS:HG3 | 1:B:127:ILE:CG2 | 0.40 | 2.47 | 10 | 1 |
| 1:A:5:THR:CG2 | 1:B:103:ARG:NE | 0.40 | 2.83 | 18 | 1 |
| 1:B:116:LEU:HG | 1:B:117:LYS:N | 0.40 | 2.32 | 16 | 1 |
| 1:A:35:LEU:HD13 | 1:B:116:LEU:HG | 0.40 | 1.94 | 7 | 1 |
| 1:B:119:LEU:HD11 | 1:B:130:TYR:CE2 | 0.40 | 2.52 | 17 | 1 |
| 1:A:34:ARG:O | 1:B:134:ARG:CG | 0.40 | 2.69 | 21 | 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 | 51/83 (61%) | 45±2 (89±4%) | 5±2 (10±4%) | 1±1 (1±2%) | 14 | 59 |
| 1 | B | 34/83 (41%) | 32±1 (95±3%) | 2±1 (5±3%) | 0±0 (0±1%) | 32 | 76 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|----------|-------------|
| All | All | 2040/3984 (51%) | 1859 (91%) | 159 (8%) | 22 (1%) | 18 66 |

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 54 | GLY | 4 |
| 1 | A | 10 | ASP | 3 |
| 1 | B | 102 | SER | 3 |
| 1 | A | 2 | SER | 2 |
| 1 | A | 52 | MET | 2 |
| 1 | A | 53 | LEU | 2 |
| 1 | A | 55 | ASN | 2 |
| 1 | B | 110 | ASP | 1 |
| 1 | A | 41 | ASP | 1 |
| 1 | A | 45 | ALA | 1 |
| 1 | A | 51 | THR | 1 |

6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|--------------|--------------|-------------|
| 1 | A | 42/67 (63%) | 25±3 (60±7%) | 17±3 (40±7%) | 0 5 |
| 1 | B | 29/67 (43%) | 16±2 (57±8%) | 13±2 (43±8%) | 0 3 |
| All | All | 1704/3216 (53%) | 998 (59%) | 706 (41%) | 0 4 |

All 62 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 19 | LEU | 24 |
| 1 | B | 104 | LEU | 24 |
| 1 | B | 119 | LEU | 24 |
| 1 | A | 17 | LYS | 23 |
| 1 | A | 8 | MET | 22 |
| 1 | B | 108 | MET | 22 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 2 | SER | 21 |
| 1 | B | 117 | LYS | 21 |
| 1 | A | 4 | LEU | 19 |
| 1 | A | 12 | GLN | 19 |
| 1 | B | 109 | THR | 19 |
| 1 | B | 134 | ARG | 18 |
| 1 | B | 128 | LYS | 18 |
| 1 | B | 102 | SER | 17 |
| 1 | B | 127 | ILE | 17 |
| 1 | A | 23 | GLN | 17 |
| 1 | A | 29 | GLN | 17 |
| 1 | A | 27 | ILE | 16 |
| 1 | A | 50 | LYS | 16 |
| 1 | B | 129 | GLN | 16 |
| 1 | A | 34 | ARG | 15 |
| 1 | A | 16 | LEU | 15 |
| 1 | A | 9 | THR | 14 |
| 1 | B | 123 | GLN | 14 |
| 1 | B | 112 | GLN | 14 |
| 1 | B | 116 | LEU | 14 |
| 1 | A | 28 | LYS | 13 |
| 1 | A | 53 | LEU | 13 |
| 1 | B | 115 | SER | 13 |
| 1 | A | 15 | SER | 13 |
| 1 | A | 25 | LYS | 12 |
| 1 | A | 47 | GLN | 12 |
| 1 | A | 49 | LEU | 11 |
| 1 | B | 111 | GLN | 10 |
| 1 | B | 125 | LYS | 9 |
| 1 | A | 43 | ASP | 8 |
| 1 | A | 46 | TRP | 8 |
| 1 | A | 52 | MET | 8 |
| 1 | A | 51 | THR | 7 |
| 1 | B | 122 | LEU | 7 |
| 1 | A | 32 | LEU | 7 |
| 1 | A | 3 | ARG | 7 |
| 1 | A | 55 | ASN | 6 |
| 1 | A | 11 | GLN | 6 |
| 1 | B | 132 | LEU | 6 |
| 1 | A | 10 | ASP | 6 |
| 1 | A | 44 | GLN | 5 |
| 1 | A | 41 | ASP | 5 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | B | 103 | ARG | 5 |
| 1 | A | 22 | LEU | 5 |
| 1 | B | 110 | ASP | 4 |
| 1 | A | 48 | GLU | 4 |
| 1 | A | 6 | ILE | 3 |
| 1 | A | 39 | ASP | 3 |
| 1 | B | 105 | THR | 3 |
| 1 | B | 106 | ILE | 2 |
| 1 | B | 135 | LEU | 2 |
| 1 | A | 35 | LEU | 2 |
| 1 | B | 130 | TYR | 2 |
| 1 | A | 5 | THR | 1 |
| 1 | B | 113 | HIS | 1 |
| 1 | A | 30 | TYR | 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 monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

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

| | |
|---|------|
| Total number of shifts | 1712 |
| Number of shifts mapped to atoms | 1712 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 18 |

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|-------------------------|
| $^{13}\text{C}_\alpha$ | 160 | -1.40 \pm 0.09 | Should be checked |
| $^{13}\text{C}_\beta$ | 146 | -0.20 \pm 0.07 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 158 | 0.91 \pm 0.33 | Should be applied |
| ^{15}N | 158 | 0.42 \pm 0.29 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 913 atoms were assigned a chemical shift out of a possible 1190. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 405/428 (95%) | 162/173 (94%) | 162/170 (95%) | 81/85 (95%) |
| Sidechain | 495/716 (69%) | 310/464 (67%) | 172/220 (78%) | 13/32 (41%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 13/46 (28%) | 12/22 (55%) | 0/19 (0%) | 1/5 (20%) |
| Overall | 913/1190 (77%) | 484/659 (73%) | 334/409 (82%) | 95/122 (78%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1712 atoms were assigned a chemical shift out of a possible 2214. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 796/840 (95%) | 320/344 (93%) | 318/332 (96%) | 158/164 (96%) |
| Sidechain | 890/1296 (69%) | 548/838 (65%) | 324/404 (80%) | 18/54 (33%) |
| Aromatic | 26/78 (33%) | 24/38 (63%) | 0/34 (0%) | 2/6 (33%) |
| Overall | 1712/2214 (77%) | 892/1220 (73%) | 642/770 (83%) | 178/224 (79%) |

7.1.4 Statistically unusual chemical shifts

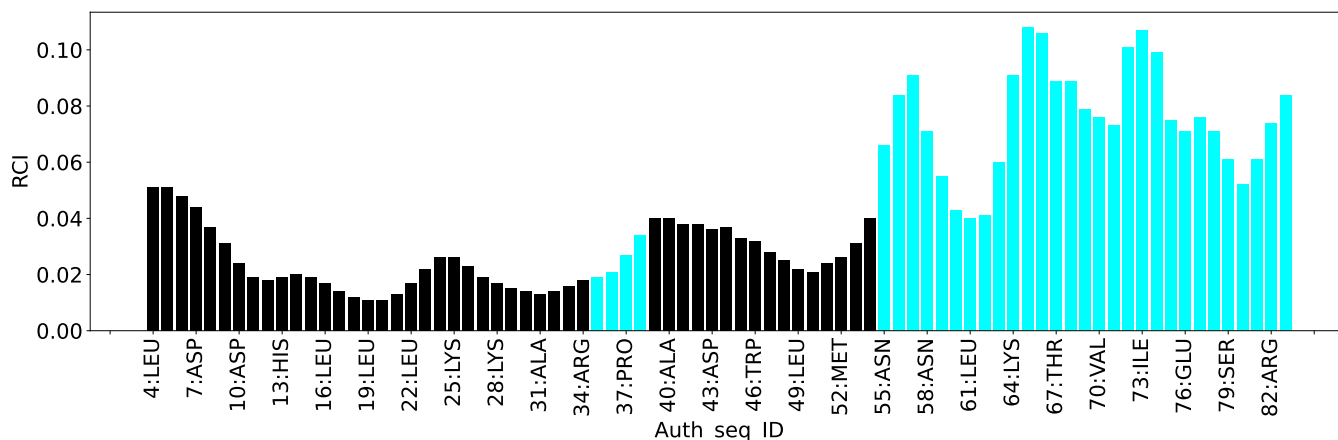
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 19 | LEU | CG | 67.09 | 21.37 – 32.19 | 37.3 |
| 1 | B | 119 | LEU | CG | 67.09 | 21.37 – 32.19 | 37.3 |
| 1 | A | 9 | THR | CG2 | 61.67 | 16.06 – 27.03 | 36.6 |
| 1 | B | 109 | THR | CG2 | 61.67 | 16.06 – 27.03 | 36.6 |
| 1 | A | 58 | ASN | CG | 112.29 | 164.52 – 188.90 | -26.4 |
| 1 | B | 158 | ASN | CG | 112.29 | 164.52 – 188.90 | -26.4 |
| 1 | A | 11 | GLN | CD | 171.82 | 173.59 – 185.85 | -6.4 |
| 1 | B | 111 | GLN | CD | 171.82 | 173.59 – 185.85 | -6.4 |
| 1 | A | 44 | GLN | CD | 171.87 | 173.59 – 185.85 | -6.4 |
| 1 | B | 144 | GLN | CD | 171.87 | 173.59 – 185.85 | -6.4 |
| 1 | A | 47 | GLN | CD | 172.04 | 173.59 – 185.85 | -6.3 |
| 1 | B | 147 | GLN | CD | 172.04 | 173.59 – 185.85 | -6.3 |
| 1 | A | 14 | GLN | CD | 172.05 | 173.59 – 185.85 | -6.2 |
| 1 | B | 114 | GLN | CD | 172.05 | 173.59 – 185.85 | -6.2 |
| 1 | A | 23 | GLN | CD | 172.28 | 173.59 – 185.85 | -6.1 |
| 1 | B | 123 | GLN | CD | 172.28 | 173.59 – 185.85 | -6.1 |
| 1 | A | 29 | GLN | CD | 172.37 | 173.59 – 185.85 | -6.0 |
| 1 | B | 129 | GLN | CD | 172.37 | 173.59 – 185.85 | -6.0 |

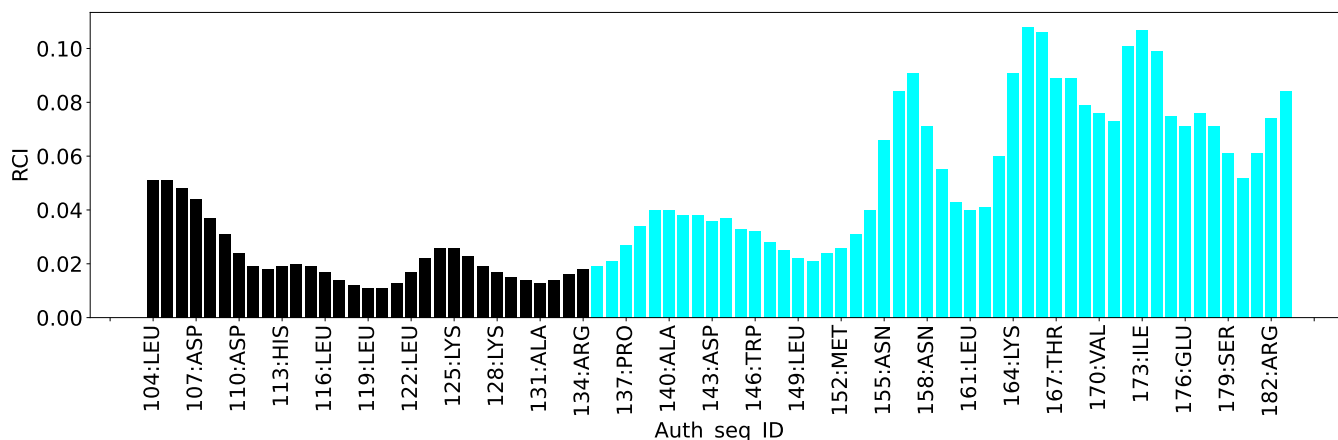
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



Random coil index (RCI) for chain B:



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 | 2108 |
| Intra-residue ($ i-j =0$) | 862 |
| Sequential ($ i-j =1$) | 498 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 300 |
| Long range ($ i-j \geq 5$) | 122 |
| Inter-chain | 326 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 0 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 12.7 |
| Number of long range restraints per residue ¹ | 0.7 |

¹Long 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) | 13.2 | 0.2 |
| 0.2-0.5 (Medium) | 1.5 | 0.42 |
| >0.5 (Large) | None | None |

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis [i](#)

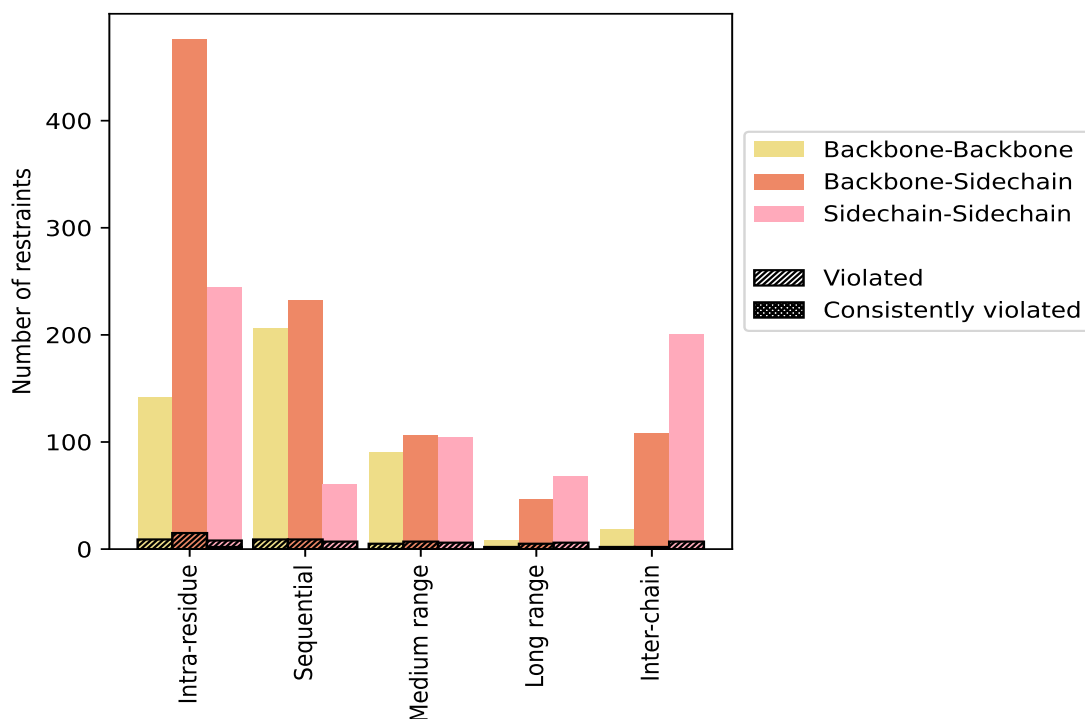
9.1 Summary of distance violations [i](#)

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 | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 862 | 40.9 | 32 | 3.7 | 1.5 | 2 | 0.2 | 0.1 |
| Backbone-Backbone | 142 | 6.7 | 9 | 6.3 | 0.4 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 476 | 22.6 | 15 | 3.2 | 0.7 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 244 | 11.6 | 8 | 3.3 | 0.4 | 2 | 0.8 | 0.1 |
| Sequential ($i-j =1$) | 498 | 23.6 | 25 | 5.0 | 1.2 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 206 | 9.8 | 9 | 4.4 | 0.4 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 232 | 11.0 | 9 | 3.9 | 0.4 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 60 | 2.8 | 7 | 11.7 | 0.3 | 0 | 0.0 | 0.0 |
| Medium range ($i-j >1$ & $i-j <5$) | 300 | 14.2 | 18 | 6.0 | 0.9 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 90 | 4.3 | 5 | 5.6 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 106 | 5.0 | 7 | 6.6 | 0.3 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 104 | 4.9 | 6 | 5.8 | 0.3 | 0 | 0.0 | 0.0 |
| Long range ($i-j \geq 5$) | 122 | 5.8 | 13 | 10.7 | 0.6 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 8 | 0.4 | 2 | 25.0 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 46 | 2.2 | 5 | 10.9 | 0.2 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 68 | 3.2 | 6 | 8.8 | 0.3 | 0 | 0.0 | 0.0 |
| Inter-chain | 326 | 15.5 | 11 | 3.4 | 0.5 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 18 | 0.9 | 2 | 11.1 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 108 | 5.1 | 2 | 1.9 | 0.1 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 200 | 9.5 | 7 | 3.5 | 0.3 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 2108 | 100.0 | 99 | 4.7 | 4.7 | 2 | 0.1 | 0.1 |
| Backbone-Backbone | 464 | 22.0 | 27 | 5.8 | 1.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 968 | 45.9 | 38 | 3.9 | 1.8 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 676 | 32.1 | 34 | 5.0 | 1.6 | 2 | 0.3 | 0.1 |

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ 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 disulfid 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 ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 3 | 2 | 0 | 0 | 1 | 6 | 0.12 | 0.13 | 0.01 | 0.12 |
| 2 | 4 | 4 | 2 | 1 | 4 | 15 | 0.13 | 0.17 | 0.02 | 0.12 |
| 3 | 10 | 4 | 8 | 2 | 1 | 25 | 0.17 | 0.34 | 0.07 | 0.13 |
| 4 | 5 | 4 | 1 | 1 | 3 | 14 | 0.14 | 0.22 | 0.03 | 0.14 |
| 5 | 6 | 5 | 2 | 5 | 2 | 20 | 0.15 | 0.35 | 0.05 | 0.14 |
| 6 | 3 | 4 | 2 | 0 | 3 | 12 | 0.13 | 0.18 | 0.02 | 0.12 |
| 7 | 6 | 3 | 0 | 0 | 1 | 10 | 0.17 | 0.42 | 0.09 | 0.15 |
| 8 | 6 | 4 | 1 | 0 | 1 | 12 | 0.17 | 0.42 | 0.08 | 0.14 |
| 9 | 4 | 1 | 0 | 1 | 2 | 8 | 0.13 | 0.14 | 0.01 | 0.12 |
| 10 | 4 | 6 | 1 | 6 | 3 | 20 | 0.16 | 0.28 | 0.06 | 0.14 |
| 11 | 3 | 5 | 3 | 2 | 3 | 16 | 0.13 | 0.16 | 0.02 | 0.12 |

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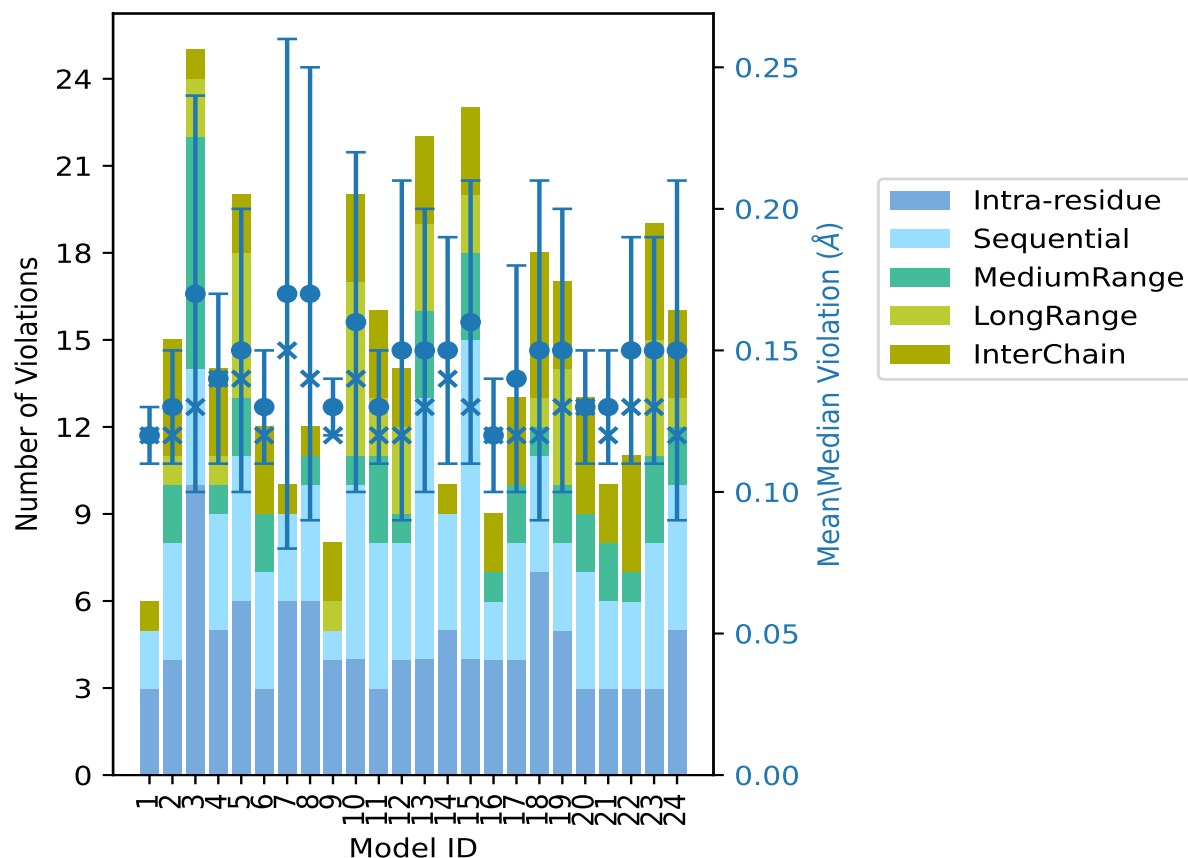
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 12 | 4 | 4 | 1 | 3 | 2 | 14 | 0.15 | 0.32 | 0.06 | 0.12 |
| 13 | 4 | 9 | 3 | 3 | 3 | 22 | 0.15 | 0.34 | 0.05 | 0.13 |
| 14 | 5 | 4 | 0 | 0 | 1 | 10 | 0.15 | 0.26 | 0.04 | 0.14 |
| 15 | 4 | 11 | 3 | 2 | 3 | 23 | 0.16 | 0.29 | 0.05 | 0.13 |
| 16 | 4 | 2 | 1 | 0 | 2 | 9 | 0.12 | 0.16 | 0.02 | 0.12 |
| 17 | 4 | 4 | 2 | 0 | 3 | 13 | 0.14 | 0.23 | 0.04 | 0.12 |
| 18 | 7 | 4 | 1 | 1 | 5 | 18 | 0.15 | 0.34 | 0.06 | 0.12 |
| 19 | 5 | 3 | 2 | 4 | 3 | 17 | 0.15 | 0.3 | 0.05 | 0.13 |
| 20 | 3 | 4 | 2 | 0 | 4 | 13 | 0.13 | 0.18 | 0.02 | 0.13 |
| 21 | 3 | 3 | 2 | 0 | 2 | 10 | 0.13 | 0.18 | 0.02 | 0.12 |
| 22 | 3 | 3 | 1 | 0 | 4 | 11 | 0.15 | 0.24 | 0.04 | 0.13 |
| 23 | 3 | 5 | 3 | 4 | 4 | 19 | 0.15 | 0.23 | 0.04 | 0.13 |
| 24 | 5 | 5 | 2 | 1 | 3 | 16 | 0.15 | 0.34 | 0.06 | 0.12 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2009(IR:830, SQ:473, MR:282, LR:109, IC:315) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 19 | 8 | 12 | 3 | 3 | 45 | 1 | 4.2 |
| 4 | 9 | 4 | 6 | 2 | 25 | 2 | 8.3 |
| 2 | 2 | 0 | 2 | 1 | 7 | 3 | 12.5 |
| 2 | 2 | 0 | 0 | 1 | 5 | 4 | 16.7 |
| 1 | 0 | 0 | 0 | 2 | 3 | 5 | 20.8 |
| 1 | 0 | 0 | 0 | 0 | 1 | 6 | 25.0 |

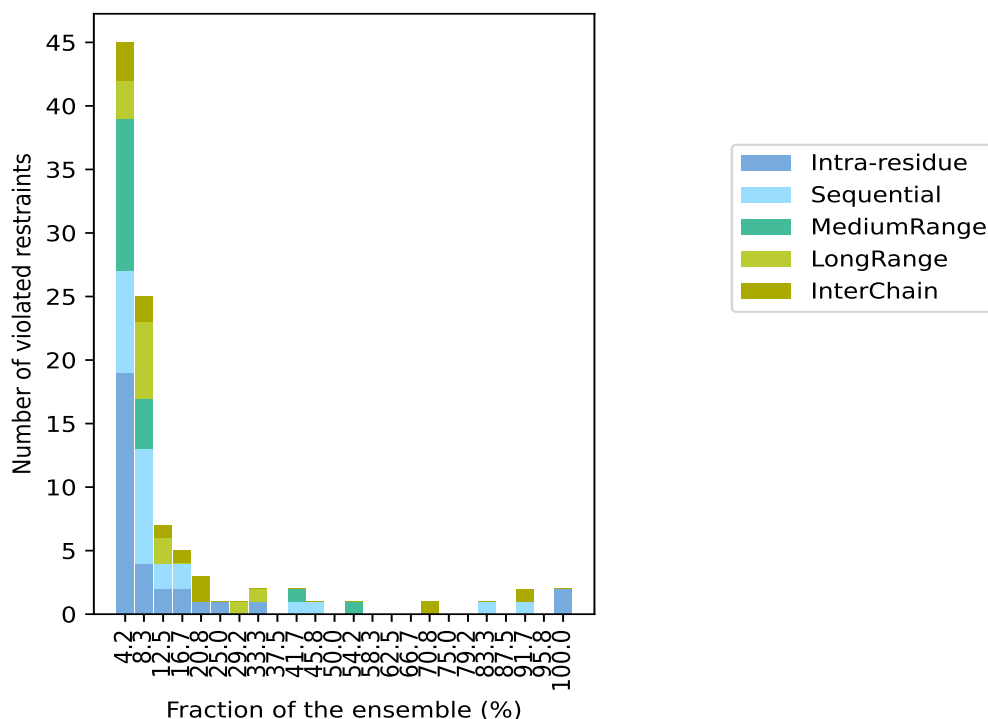
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 0 | 0 | 1 | 0 | 1 | 7 | 29.2 |
| 1 | 0 | 0 | 1 | 0 | 2 | 8 | 33.3 |
| 0 | 0 | 0 | 0 | 0 | 0 | 9 | 37.5 |
| 0 | 1 | 1 | 0 | 0 | 2 | 10 | 41.7 |
| 0 | 1 | 0 | 0 | 0 | 1 | 11 | 45.8 |
| 0 | 0 | 0 | 0 | 0 | 0 | 12 | 50.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 13 | 54.2 |
| 0 | 0 | 0 | 0 | 0 | 0 | 14 | 58.3 |
| 0 | 0 | 0 | 0 | 0 | 0 | 15 | 62.5 |
| 0 | 0 | 0 | 0 | 0 | 0 | 16 | 66.7 |
| 0 | 0 | 0 | 0 | 1 | 1 | 17 | 70.8 |
| 0 | 0 | 0 | 0 | 0 | 0 | 18 | 75.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 19 | 79.2 |
| 0 | 1 | 0 | 0 | 0 | 1 | 20 | 83.3 |
| 0 | 0 | 0 | 0 | 0 | 0 | 21 | 87.5 |
| 0 | 1 | 0 | 0 | 1 | 2 | 22 | 91.7 |
| 0 | 0 | 0 | 0 | 0 | 0 | 23 | 95.8 |
| 2 | 0 | 0 | 0 | 0 | 2 | 24 | 100.0 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

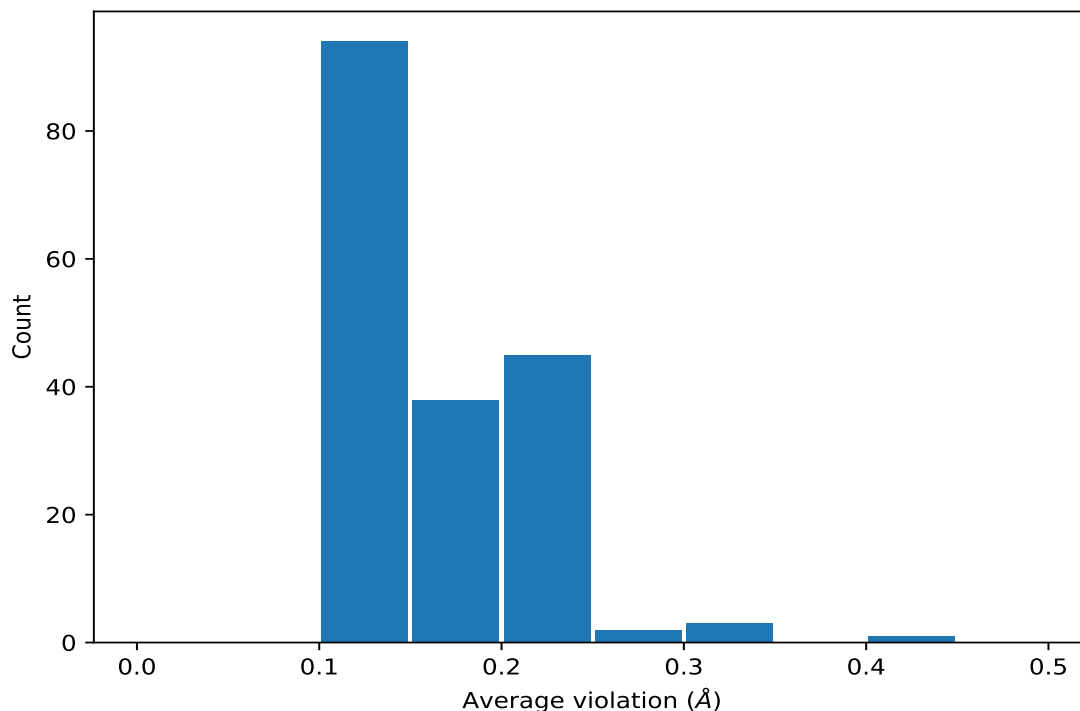
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 24 | 0.12 | 0.0 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 24 | 0.12 | 0.0 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 24 | 0.12 | 0.0 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 24 | 0.12 | 0.0 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 22 | 0.16 | 0.03 | 0.15 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 22 | 0.16 | 0.03 | 0.15 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 22 | 0.16 | 0.03 | 0.15 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 22 | 0.16 | 0.03 | 0.15 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 22 | 0.16 | 0.03 | 0.15 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 22 | 0.16 | 0.03 | 0.15 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 22 | 0.16 | 0.03 | 0.15 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 22 | 0.16 | 0.03 | 0.15 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 22 | 0.16 | 0.03 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 22 | 0.14 | 0.02 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 22 | 0.14 | 0.02 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 22 | 0.14 | 0.02 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 22 | 0.14 | 0.02 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 20 | 0.14 | 0.03 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 20 | 0.14 | 0.03 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 20 | 0.14 | 0.03 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 20 | 0.14 | 0.03 | 0.13 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 17 | 0.16 | 0.03 | 0.15 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 17 | 0.16 | 0.03 | 0.15 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 17 | 0.16 | 0.03 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 17 | 0.16 | 0.03 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 17 | 0.16 | 0.03 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 17 | 0.16 | 0.03 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 17 | 0.16 | 0.03 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 17 | 0.16 | 0.03 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 17 | 0.16 | 0.03 | 0.15 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 13 | 0.13 | 0.02 | 0.13 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 11 | 0.13 | 0.02 | 0.12 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 10 | 0.14 | 0.02 | 0.14 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 10 | 0.12 | 0.01 | 0.12 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 8 | 0.23 | 0.06 | 0.22 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 8 | 0.23 | 0.06 | 0.22 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 8 | 0.23 | 0.06 | 0.22 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 8 | 0.23 | 0.06 | 0.22 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 8 | 0.23 | 0.06 | 0.22 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 8 | 0.23 | 0.06 | 0.22 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 8 | 0.12 | 0.01 | 0.11 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG12 | 7 | 0.18 | 0.04 | 0.17 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG13 | 7 | 0.18 | 0.04 | 0.17 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG12 | 7 | 0.18 | 0.04 | 0.17 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG13 | 7 | 0.18 | 0.04 | 0.17 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG12 | 7 | 0.18 | 0.04 | 0.17 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG13 | 7 | 0.18 | 0.04 | 0.17 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB2 | 6 | 0.15 | 0.05 | 0.14 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB3 | 6 | 0.15 | 0.05 | 0.14 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB2 | 6 | 0.15 | 0.05 | 0.14 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB3 | 6 | 0.15 | 0.05 | 0.14 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB2 | 6 | 0.15 | 0.05 | 0.14 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB3 | 6 | 0.15 | 0.05 | 0.14 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD1 | 5 | 0.13 | 0.03 | 0.12 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD2 | 5 | 0.13 | 0.03 | 0.12 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD1 | 5 | 0.13 | 0.03 | 0.12 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD2 | 5 | 0.13 | 0.03 | 0.12 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD1 | 5 | 0.13 | 0.03 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD2 | 5 | 0.13 | 0.03 | 0.12 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB3 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB3 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB3 | 5 | 0.13 | 0.02 | 0.12 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD1 | 5 | 0.11 | 0.0 | 0.11 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD2 | 5 | 0.11 | 0.0 | 0.11 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD1 | 5 | 0.11 | 0.0 | 0.11 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD2 | 5 | 0.11 | 0.0 | 0.11 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD1 | 5 | 0.11 | 0.0 | 0.11 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD2 | 5 | 0.11 | 0.0 | 0.11 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD11 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD12 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD13 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD21 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD22 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD23 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD11 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD12 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD13 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD21 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD22 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD23 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD11 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD12 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD13 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD21 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD22 | 4 | 0.23 | 0.05 | 0.24 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD23 | 4 | 0.23 | 0.05 | 0.24 |
| (1,196) | 1:A:17:LYS:HD2 | 1:A:18:ALA:H | 4 | 0.22 | 0.1 | 0.22 |
| (1,196) | 1:A:17:LYS:HD3 | 1:A:18:ALA:H | 4 | 0.22 | 0.1 | 0.22 |
| (1,222) | 1:A:19:LEU:HA | 1:A:19:LEU:HG | 4 | 0.15 | 0.02 | 0.15 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG21 | 4 | 0.12 | 0.01 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG22 | 4 | 0.12 | 0.01 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG23 | 4 | 0.12 | 0.01 | 0.11 |
| (1,589) | 1:A:40:ALA:H | 1:A:40:ALA:HA | 4 | 0.11 | 0.0 | 0.11 |
| (1,33) | 1:A:6:ILE:HD11 | 1:A:6:ILE:HB | 3 | 0.34 | 0.0 | 0.34 |
| (1,33) | 1:A:6:ILE:HD12 | 1:A:6:ILE:HB | 3 | 0.34 | 0.0 | 0.34 |
| (1,33) | 1:A:6:ILE:HD13 | 1:A:6:ILE:HB | 3 | 0.34 | 0.0 | 0.34 |
| (1,1250) | 1:B:117:LYS:HD2 | 1:B:118:ALA:H | 3 | 0.25 | 0.07 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1250) | 1:B:117:LYS:HD3 | 1:B:118:ALA:H | 3 | 0.25 | 0.07 | 0.27 |
| (1,1185) | 1:B:113:HIS:HD2 | 1:B:127:ILE:HB | 3 | 0.21 | 0.03 | 0.23 |
| (1,1339) | 1:B:122:LEU:HA | 1:B:122:LEU:HG | 3 | 0.15 | 0.0 | 0.15 |
| (1,1220) | 1:B:116:LEU:HB2 | 1:B:117:LYS:H | 3 | 0.14 | 0.01 | 0.14 |
| (1,1220) | 1:B:116:LEU:HB3 | 1:B:117:LYS:H | 3 | 0.14 | 0.01 | 0.14 |
| (1,2079) | 1:B:131:ALA:HA | 1:A:35:LEU:H | 3 | 0.12 | 0.01 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG21 | 1:B:117:LYS:HA | 3 | 0.11 | 0.0 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG22 | 1:B:117:LYS:HA | 3 | 0.11 | 0.0 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG23 | 1:B:117:LYS:HA | 3 | 0.11 | 0.0 | 0.11 |
| (1,739) | 1:A:53:LEU:H | 1:A:53:LEU:HG | 2 | 0.42 | 0.0 | 0.42 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD11 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD12 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD13 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD21 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD22 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD23 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD11 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD12 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD13 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD21 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD22 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD23 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD11 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD12 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD13 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD21 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD22 | 2 | 0.2 | 0.03 | 0.2 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD23 | 2 | 0.2 | 0.03 | 0.2 |
| (1,131) | 1:A:13:HIS:HD2 | 1:A:27:ILE:HB | 2 | 0.18 | 0.01 | 0.18 |
| (1,280) | 1:A:22:LEU:HA | 1:A:21:ALA:H | 2 | 0.18 | 0.0 | 0.18 |
| (1,1753) | 1:B:149:LEU:HA | 1:B:152:MET:HB2 | 2 | 0.18 | 0.05 | 0.18 |
| (1,1753) | 1:B:149:LEU:HA | 1:B:152:MET:HB3 | 2 | 0.18 | 0.05 | 0.18 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD11 | 2 | 0.17 | 0.0 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD12 | 2 | 0.17 | 0.0 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD13 | 2 | 0.17 | 0.0 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD21 | 2 | 0.17 | 0.0 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD22 | 2 | 0.17 | 0.0 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD23 | 2 | 0.17 | 0.0 | 0.17 |
| (1,1741) | 1:B:148:GLU:HA | 1:B:151:THR:HA | 2 | 0.16 | 0.03 | 0.16 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB3 | 2 | 0.16 | 0.02 | 0.16 |

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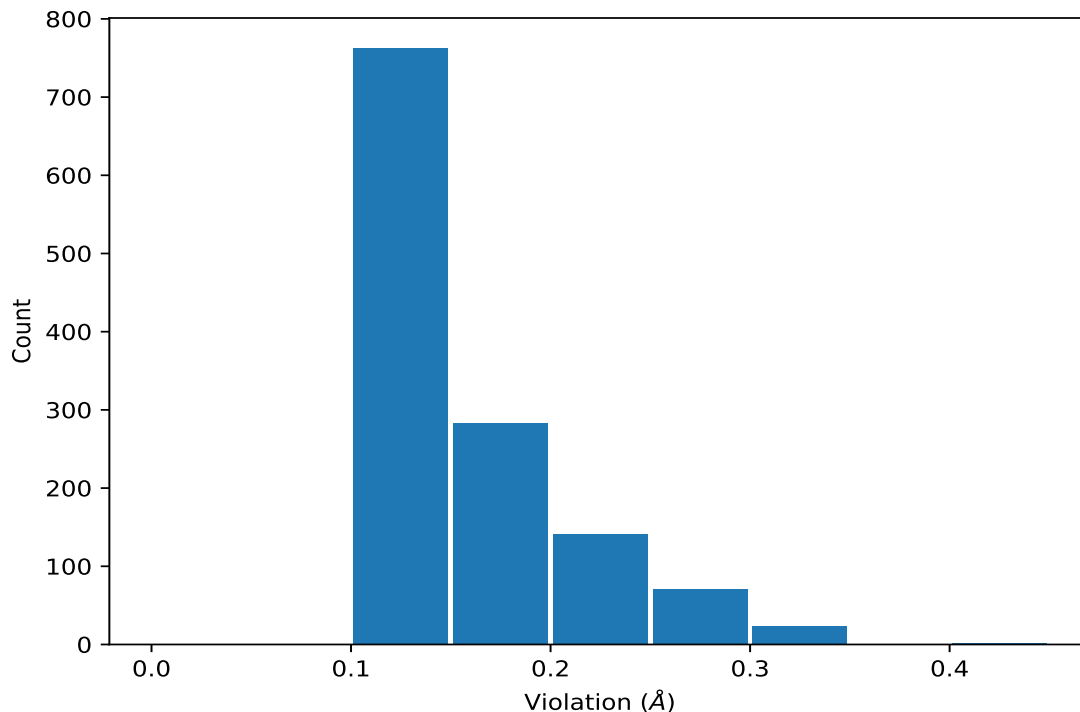
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,968) | 1:A:8:MET:HE1 | 1:B:104:LEU:H | 2 | 0.15 | 0.02 | 0.15 |
| (1,968) | 1:A:8:MET:HE2 | 1:B:104:LEU:H | 2 | 0.15 | 0.02 | 0.15 |
| (1,968) | 1:A:8:MET:HE3 | 1:B:104:LEU:H | 2 | 0.15 | 0.02 | 0.15 |
| (1,285) | 1:A:22:LEU:HA | 1:A:22:LEU:HG | 2 | 0.15 | 0.0 | 0.15 |
| (1,362) | 1:A:27:ILE:HD11 | 1:A:17:LYS:HG2 | 2 | 0.14 | 0.03 | 0.14 |
| (1,362) | 1:A:27:ILE:HD11 | 1:A:17:LYS:HG3 | 2 | 0.14 | 0.03 | 0.14 |
| (1,362) | 1:A:27:ILE:HD12 | 1:A:17:LYS:HG2 | 2 | 0.14 | 0.03 | 0.14 |
| (1,362) | 1:A:27:ILE:HD12 | 1:A:17:LYS:HG3 | 2 | 0.14 | 0.03 | 0.14 |
| (1,362) | 1:A:27:ILE:HD13 | 1:A:17:LYS:HG2 | 2 | 0.14 | 0.03 | 0.14 |
| (1,362) | 1:A:27:ILE:HD13 | 1:A:17:LYS:HG3 | 2 | 0.14 | 0.03 | 0.14 |
| (1,1415) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1415) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,1415) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HA | 2 | 0.14 | 0.0 | 0.14 |
| (1,637) | 1:A:45:ALA:HB1 | 1:A:46:TRP:HD1 | 2 | 0.14 | 0.01 | 0.14 |
| (1,637) | 1:A:45:ALA:HB2 | 1:A:46:TRP:HD1 | 2 | 0.14 | 0.01 | 0.14 |
| (1,637) | 1:A:45:ALA:HB3 | 1:A:46:TRP:HD1 | 2 | 0.14 | 0.01 | 0.14 |
| (1,365) | 1:A:27:ILE:HG21 | 1:A:17:LYS:HA | 2 | 0.13 | 0.0 | 0.13 |
| (1,365) | 1:A:27:ILE:HG22 | 1:A:17:LYS:HA | 2 | 0.13 | 0.0 | 0.13 |
| (1,365) | 1:A:27:ILE:HG23 | 1:A:17:LYS:HA | 2 | 0.13 | 0.0 | 0.13 |
| (1,547) | 1:A:35:LEU:H | 1:A:36:PHE:HA | 2 | 0.13 | 0.01 | 0.13 |
| (1,1120) | 1:B:108:MET:HG2 | 1:B:106:ILE:HG12 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1120) | 1:B:108:MET:HG2 | 1:B:106:ILE:HG13 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1120) | 1:B:108:MET:HG3 | 1:B:106:ILE:HG12 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1120) | 1:B:108:MET:HG3 | 1:B:106:ILE:HG13 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1601) | 1:B:135:LEU:H | 1:B:136:PHE:HA | 2 | 0.12 | 0.01 | 0.12 |
| (1,1204) | 1:B:114:GLN:H | 1:B:115:SER:HA | 2 | 0.12 | 0.01 | 0.12 |
| (1,1315) | 1:B:120:ALA:HA | 1:B:131:ALA:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,610) | 1:A:43:ASP:H | 1:A:43:ASP:HA | 2 | 0.12 | 0.0 | 0.12 |
| (1,1025) | 1:A:31:ALA:HA | 1:B:135:LEU:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,1583) | 1:B:134:ARG:H | 1:B:133:GLU:HA | 2 | 0.12 | 0.0 | 0.12 |
| (1,180) | 1:A:16:LEU:H | 1:A:19:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,180) | 1:A:16:LEU:H | 1:A:19:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HG2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HG3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HG2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HG3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HG2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HG3 | 2 | 0.11 | 0.0 | 0.11 |

¹Number of violated models, ²Standard 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) |
|----------|-----------------|------------------|----------|---------------|
| (1,739) | 1:A:53:LEU:H | 1:A:53:LEU:HG | 7 | 0.42 |
| (1,739) | 1:A:53:LEU:H | 1:A:53:LEU:HG | 8 | 0.42 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 5 | 0.35 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 5 | 0.35 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 5 | 0.35 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 5 | 0.35 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 5 | 0.35 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 5 | 0.35 |
| (1,33) | 1:A:6:ILE:HD11 | 1:A:6:ILE:HB | 18 | 0.34 |
| (1,33) | 1:A:6:ILE:HD12 | 1:A:6:ILE:HB | 18 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,33) | 1:A:6:ILE:HD13 | 1:A:6:ILE:HB | 18 | 0.34 |
| (1,33) | 1:A:6:ILE:HD11 | 1:A:6:ILE:HB | 24 | 0.34 |
| (1,33) | 1:A:6:ILE:HD12 | 1:A:6:ILE:HB | 24 | 0.34 |
| (1,33) | 1:A:6:ILE:HD13 | 1:A:6:ILE:HB | 24 | 0.34 |
| (1,196) | 1:A:17:LYS:HD2 | 1:A:18:ALA:H | 13 | 0.34 |
| (1,196) | 1:A:17:LYS:HD3 | 1:A:18:ALA:H | 13 | 0.34 |
| (1,1640) | 1:B:140:ALA:HA | 1:B:143:ASP:HB2 | 3 | 0.34 |
| (1,1640) | 1:B:140:ALA:HA | 1:B:143:ASP:HB3 | 3 | 0.34 |
| (1,33) | 1:A:6:ILE:HD11 | 1:A:6:ILE:HB | 3 | 0.33 |
| (1,33) | 1:A:6:ILE:HD12 | 1:A:6:ILE:HB | 3 | 0.33 |
| (1,33) | 1:A:6:ILE:HD13 | 1:A:6:ILE:HB | 3 | 0.33 |
| (1,1087) | 1:B:106:ILE:HD11 | 1:B:106:ILE:HB | 3 | 0.33 |
| (1,1087) | 1:B:106:ILE:HD12 | 1:B:106:ILE:HB | 3 | 0.33 |
| (1,1087) | 1:B:106:ILE:HD13 | 1:B:106:ILE:HB | 3 | 0.33 |
| (1,1250) | 1:B:117:LYS:HD2 | 1:B:118:ALA:H | 12 | 0.32 |
| (1,1250) | 1:B:117:LYS:HD3 | 1:B:118:ALA:H | 12 | 0.32 |
| (1,196) | 1:A:17:LYS:HD2 | 1:A:18:ALA:H | 19 | 0.3 |
| (1,196) | 1:A:17:LYS:HD3 | 1:A:18:ALA:H | 19 | 0.3 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD11 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD12 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD13 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD21 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD22 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD23 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD11 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD12 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD13 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD21 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD22 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD23 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD11 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD12 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD13 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD21 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD22 | 15 | 0.29 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD23 | 15 | 0.29 |
| (1,1867) | 1:B:170:VAL:H | 1:B:170:VAL:HG21 | 3 | 0.28 |
| (1,1867) | 1:B:170:VAL:H | 1:B:170:VAL:HG22 | 3 | 0.28 |
| (1,1867) | 1:B:170:VAL:H | 1:B:170:VAL:HG23 | 3 | 0.28 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 10 | 0.28 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 10 | 0.28 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 10 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 10 | 0.28 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 10 | 0.28 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 10 | 0.28 |
| (1,1250) | 1:B:117:LYS:HD2 | 1:B:118:ALA:H | 10 | 0.27 |
| (1,1250) | 1:B:117:LYS:HD3 | 1:B:118:ALA:H | 10 | 0.27 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD11 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD12 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD13 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD21 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD22 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD23 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD11 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD12 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD13 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD21 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD22 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD23 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD11 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD12 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD13 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD21 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD22 | 14 | 0.26 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD23 | 14 | 0.26 |
| (1,1661) | 1:B:143:ASP:H | 1:B:141:ASP:H | 3 | 0.26 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 10 | 0.25 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 10 | 0.25 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 10 | 0.25 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 10 | 0.25 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 10 | 0.25 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 10 | 0.25 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 10 | 0.25 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 10 | 0.25 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 10 | 0.25 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB2 | 18 | 0.25 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB3 | 18 | 0.25 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB2 | 18 | 0.25 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB3 | 18 | 0.25 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB2 | 18 | 0.25 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB3 | 18 | 0.25 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 12 | 0.25 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 12 | 0.25 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 12 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 12 | 0.25 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 12 | 0.25 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 12 | 0.25 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD11 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD12 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD13 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD21 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD22 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD23 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD11 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD12 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD13 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD21 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD22 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD23 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD11 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD12 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD13 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD21 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD22 | 22 | 0.24 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD23 | 22 | 0.24 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG12 | 19 | 0.24 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG13 | 19 | 0.24 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG12 | 19 | 0.24 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG13 | 19 | 0.24 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG12 | 19 | 0.24 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG13 | 19 | 0.24 |
| (1,1185) | 1:B:113:HIS:HD2 | 1:B:127:ILE:HB | 10 | 0.24 |
| (1,540) | 1:A:35:LEU:HG | 1:A:35:LEU:H | 15 | 0.23 |
| (1,1753) | 1:B:149:LEU:HA | 1:B:152:MET:HB2 | 3 | 0.23 |
| (1,1753) | 1:B:149:LEU:HA | 1:B:152:MET:HB3 | 3 | 0.23 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 23 | 0.23 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 23 | 0.23 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 23 | 0.23 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 23 | 0.23 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 23 | 0.23 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 23 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB1 | 1:B:119:LEU:HD11 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB1 | 1:B:119:LEU:HD12 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB1 | 1:B:119:LEU:HD13 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB1 | 1:B:119:LEU:HD21 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB1 | 1:B:119:LEU:HD22 | 17 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1263) | 1:B:118:ALA:HB1 | 1:B:119:LEU:HD23 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB2 | 1:B:119:LEU:HD11 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB2 | 1:B:119:LEU:HD12 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB2 | 1:B:119:LEU:HD13 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB2 | 1:B:119:LEU:HD21 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB2 | 1:B:119:LEU:HD22 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB2 | 1:B:119:LEU:HD23 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB3 | 1:B:119:LEU:HD11 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB3 | 1:B:119:LEU:HD12 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB3 | 1:B:119:LEU:HD13 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB3 | 1:B:119:LEU:HD21 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB3 | 1:B:119:LEU:HD22 | 17 | 0.23 |
| (1,1263) | 1:B:118:ALA:HB3 | 1:B:119:LEU:HD23 | 17 | 0.23 |
| (1,1185) | 1:B:113:HIS:HD2 | 1:B:127:ILE:HB | 5 | 0.23 |
| (1,544) | 1:A:35:LEU:HG | 1:A:36:PHE:H | 15 | 0.22 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG12 | 15 | 0.22 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG13 | 15 | 0.22 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG12 | 15 | 0.22 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG13 | 15 | 0.22 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG12 | 15 | 0.22 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG13 | 15 | 0.22 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD11 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD12 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD13 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD21 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD22 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD23 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD11 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD12 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD13 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD21 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD22 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD23 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD11 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD12 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD13 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD21 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD22 | 4 | 0.22 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD23 | 4 | 0.22 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 18 | 0.22 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 18 | 0.22 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 18 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 18 | 0.22 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 18 | 0.22 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 18 | 0.22 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 18 | 0.22 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 18 | 0.22 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 18 | 0.22 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 24 | 0.22 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 24 | 0.22 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 24 | 0.22 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 24 | 0.22 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 24 | 0.22 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 24 | 0.22 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 24 | 0.22 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 24 | 0.22 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 24 | 0.22 |
| (1,1594) | 1:B:135:LEU:HG | 1:B:135:LEU:H | 8 | 0.22 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 15 | 0.21 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 15 | 0.21 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 15 | 0.21 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 15 | 0.21 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 15 | 0.21 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 15 | 0.21 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 15 | 0.21 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 15 | 0.21 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 15 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 13 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 13 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 13 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 13 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 13 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 13 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 24 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 24 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 24 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 24 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 24 | 0.21 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 24 | 0.21 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 22 | 0.2 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 22 | 0.2 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 22 | 0.2 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 22 | 0.2 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 22 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 22 | 0.2 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 22 | 0.2 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 22 | 0.2 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 22 | 0.2 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 23 | 0.2 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 23 | 0.2 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 23 | 0.2 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 23 | 0.2 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 23 | 0.2 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 23 | 0.2 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 23 | 0.2 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 23 | 0.2 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 23 | 0.2 |
| (1,1879) | 1:B:173:ILE:HD11 | 1:B:173:ILE:HA | 10 | 0.2 |
| (1,1879) | 1:B:173:ILE:HD12 | 1:B:173:ILE:HA | 10 | 0.2 |
| (1,1879) | 1:B:173:ILE:HD13 | 1:B:173:ILE:HA | 10 | 0.2 |
| (1,1248) | 1:B:117:LYS:HD2 | 1:B:117:LYS:H | 5 | 0.2 |
| (1,1248) | 1:B:117:LYS:HD3 | 1:B:117:LYS:H | 5 | 0.2 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD1 | 23 | 0.19 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD2 | 23 | 0.19 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD1 | 23 | 0.19 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD2 | 23 | 0.19 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD1 | 23 | 0.19 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD2 | 23 | 0.19 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 4 | 0.19 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 4 | 0.19 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 4 | 0.19 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 4 | 0.19 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 18 | 0.19 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 18 | 0.19 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 18 | 0.19 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 18 | 0.19 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 24 | 0.19 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 24 | 0.19 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 24 | 0.19 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 24 | 0.19 |
| (1,378) | 1:A:27:ILE:HG21 | 1:A:30:TYR:HD1 | 13 | 0.19 |
| (1,378) | 1:A:27:ILE:HG21 | 1:A:30:TYR:HD2 | 13 | 0.19 |
| (1,378) | 1:A:27:ILE:HG22 | 1:A:30:TYR:HD1 | 13 | 0.19 |
| (1,378) | 1:A:27:ILE:HG22 | 1:A:30:TYR:HD2 | 13 | 0.19 |
| (1,378) | 1:A:27:ILE:HG23 | 1:A:30:TYR:HD1 | 13 | 0.19 |
| (1,378) | 1:A:27:ILE:HG23 | 1:A:30:TYR:HD2 | 13 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG12 | 13 | 0.19 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG13 | 13 | 0.19 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG12 | 13 | 0.19 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG13 | 13 | 0.19 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG12 | 13 | 0.19 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG13 | 13 | 0.19 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 23 | 0.19 |
| (1,1741) | 1:B:148:GLU:HA | 1:B:151:THR:HA | 3 | 0.19 |
| (1,131) | 1:A:13:HIS:HD2 | 1:A:27:ILE:HB | 19 | 0.19 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 6 | 0.18 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 6 | 0.18 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 6 | 0.18 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 6 | 0.18 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 6 | 0.18 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 6 | 0.18 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 6 | 0.18 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 6 | 0.18 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 6 | 0.18 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 7 | 0.18 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 7 | 0.18 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 7 | 0.18 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 7 | 0.18 |
| (1,280) | 1:A:22:LEU:HA | 1:A:21:ALA:H | 15 | 0.18 |
| (1,280) | 1:A:22:LEU:HA | 1:A:21:ALA:H | 22 | 0.18 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 20 | 0.18 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 20 | 0.18 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 20 | 0.18 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 20 | 0.18 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 20 | 0.18 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 20 | 0.18 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 20 | 0.18 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 20 | 0.18 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 20 | 0.18 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB1 | 3 | 0.18 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB2 | 3 | 0.18 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB3 | 3 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 8 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 8 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 8 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 8 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 17 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 17 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 17 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 21 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 21 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 21 | 0.18 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 21 | 0.18 |
| (1,131) | 1:A:13:HIS:HD2 | 1:A:27:ILE:HB | 13 | 0.18 |
| (1,1276) | 1:B:119:LEU:HA | 1:B:119:LEU:HG | 17 | 0.18 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 19 | 0.17 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 19 | 0.17 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 19 | 0.17 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 19 | 0.17 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 19 | 0.17 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 19 | 0.17 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 19 | 0.17 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 19 | 0.17 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 19 | 0.17 |
| (1,968) | 1:A:8:MET:HE1 | 1:B:104:LEU:H | 23 | 0.17 |
| (1,968) | 1:A:8:MET:HE2 | 1:B:104:LEU:H | 23 | 0.17 |
| (1,968) | 1:A:8:MET:HE3 | 1:B:104:LEU:H | 23 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD11 | 7 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD12 | 7 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD13 | 7 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD21 | 7 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD22 | 7 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD23 | 7 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD11 | 8 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD12 | 8 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD13 | 8 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD21 | 8 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD22 | 8 | 0.17 |
| (1,738) | 1:A:53:LEU:H | 1:A:53:LEU:HD23 | 8 | 0.17 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 13 | 0.17 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 5 | 0.17 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 5 | 0.17 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 5 | 0.17 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 5 | 0.17 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 14 | 0.17 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 14 | 0.17 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 14 | 0.17 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 14 | 0.17 |
| (1,362) | 1:A:27:ILE:HD11 | 1:A:17:LYS:HG2 | 18 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,362) | 1:A:27:ILE:HD11 | 1:A:17:LYS:HG3 | 18 | 0.17 |
| (1,362) | 1:A:27:ILE:HD12 | 1:A:17:LYS:HG2 | 18 | 0.17 |
| (1,362) | 1:A:27:ILE:HD12 | 1:A:17:LYS:HG3 | 18 | 0.17 |
| (1,362) | 1:A:27:ILE:HD13 | 1:A:17:LYS:HG2 | 18 | 0.17 |
| (1,362) | 1:A:27:ILE:HD13 | 1:A:17:LYS:HG3 | 18 | 0.17 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD11 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD12 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD13 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD21 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD22 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB1 | 1:A:22:LEU:HD23 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD11 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD12 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD13 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD21 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD22 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB2 | 1:A:22:LEU:HD23 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD11 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD12 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD13 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD21 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD22 | 15 | 0.17 |
| (1,273) | 1:A:21:ALA:HB3 | 1:A:22:LEU:HD23 | 15 | 0.17 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG12 | 23 | 0.17 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG13 | 23 | 0.17 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG12 | 23 | 0.17 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG13 | 23 | 0.17 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG12 | 23 | 0.17 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG13 | 23 | 0.17 |
| (1,222) | 1:A:19:LEU:HA | 1:A:19:LEU:HG | 14 | 0.17 |
| (1,222) | 1:A:19:LEU:HA | 1:A:19:LEU:HG | 15 | 0.17 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 2 | 0.17 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 12 | 0.17 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 12 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 12 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 12 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 12 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 12 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 12 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 12 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 12 | 0.17 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 21 | 0.17 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 21 | 0.17 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 21 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 21 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 21 | 0.17 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 21 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 21 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 21 | 0.17 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 21 | 0.17 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 5 | 0.17 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 10 | 0.17 |
| (1,1185) | 1:B:113:HIS:HD2 | 1:B:127:ILE:HB | 12 | 0.17 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB2 | 2 | 0.17 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB3 | 2 | 0.17 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB2 | 2 | 0.17 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB3 | 2 | 0.17 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB2 | 2 | 0.17 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB3 | 2 | 0.17 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 4 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 17 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 17 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 17 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 17 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 17 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 17 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 17 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 17 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|------------------|----------|---------------|
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 17 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 18 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 22 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 22 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 22 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 22 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 22 | 0.16 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 22 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 22 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 22 | 0.16 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 22 | 0.16 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB2 | 23 | 0.16 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB3 | 23 | 0.16 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB2 | 23 | 0.16 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB3 | 23 | 0.16 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB2 | 23 | 0.16 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB3 | 23 | 0.16 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 11 | 0.16 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG12 | 2 | 0.16 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG13 | 2 | 0.16 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG12 | 2 | 0.16 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG13 | 2 | 0.16 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG12 | 2 | 0.16 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG13 | 2 | 0.16 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD11 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD12 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD13 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD21 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD22 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB1 | 1:A:19:LEU:HD23 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD11 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD12 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD13 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD21 | 13 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD22 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB2 | 1:A:19:LEU:HD23 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD11 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD12 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD13 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD21 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD22 | 13 | 0.16 |
| (1,209) | 1:A:18:ALA:HB3 | 1:A:19:LEU:HD23 | 13 | 0.16 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 4 | 0.16 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 14 | 0.16 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 14 | 0.16 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 14 | 0.16 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 14 | 0.16 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 14 | 0.16 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 14 | 0.16 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 14 | 0.16 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 14 | 0.16 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 14 | 0.16 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 13 | 0.16 |
| (1,1572) | 1:B:134:ARG:HA | 1:B:136:PHE:HB2 | 8 | 0.16 |
| (1,1572) | 1:B:134:ARG:HA | 1:B:136:PHE:HB3 | 8 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 3 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 3 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 3 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 3 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 16 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 16 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 16 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 16 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 23 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 23 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 23 | 0.16 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 23 | 0.16 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 3 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 3 | 0.16 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 3 | 0.16 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 3 | 0.16 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 3 | 0.16 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 3 | 0.16 |
| (1,1250) | 1:B:117:LYS:HD2 | 1:B:118:ALA:H | 5 | 0.16 |
| (1,1250) | 1:B:117:LYS:HD3 | 1:B:118:ALA:H | 5 | 0.16 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 11 | 0.15 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 12 | 0.15 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 12 | 0.15 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 12 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 12 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 12 | 0.15 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 12 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 12 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 12 | 0.15 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 12 | 0.15 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 4 | 0.15 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 10 | 0.15 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 15 | 0.15 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 10 | 0.15 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 10 | 0.15 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 10 | 0.15 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 10 | 0.15 |
| (1,285) | 1:A:22:LEU:HA | 1:A:22:LEU:HG | 14 | 0.15 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG12 | 5 | 0.15 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG13 | 5 | 0.15 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG12 | 5 | 0.15 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG13 | 5 | 0.15 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG12 | 5 | 0.15 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG13 | 5 | 0.15 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 7 | 0.15 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 7 | 0.15 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 7 | 0.15 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 7 | 0.15 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 7 | 0.15 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 7 | 0.15 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 7 | 0.15 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 7 | 0.15 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 15 | 0.15 |
| (1,1890) | 1:B:173:ILE:H | 1:B:173:ILE:HG12 | 10 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 7 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 7 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 7 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 7 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 11 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 11 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 11 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 11 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 24 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 24 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 24 | 0.15 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 24 | 0.15 |
| (1,1339) | 1:B:122:LEU:HA | 1:B:122:LEU:HG | 2 | 0.15 |
| (1,1339) | 1:B:122:LEU:HA | 1:B:122:LEU:HG | 13 | 0.15 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG12 | 4 | 0.15 |
| (1,1305) | 1:B:120:ALA:HB1 | 1:B:127:ILE:HG13 | 4 | 0.15 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG12 | 4 | 0.15 |
| (1,1305) | 1:B:120:ALA:HB2 | 1:B:127:ILE:HG13 | 4 | 0.15 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG12 | 4 | 0.15 |
| (1,1305) | 1:B:120:ALA:HB3 | 1:B:127:ILE:HG13 | 4 | 0.15 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 23 | 0.15 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 24 | 0.15 |
| (1,1220) | 1:B:116:LEU:HB2 | 1:B:117:LYS:H | 24 | 0.15 |
| (1,1220) | 1:B:116:LEU:HB3 | 1:B:117:LYS:H | 24 | 0.15 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 5 | 0.14 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 20 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 20 | 0.14 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 20 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 20 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 20 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 20 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 20 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 20 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 20 | 0.14 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 21 | 0.14 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 21 | 0.14 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 21 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 21 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 21 | 0.14 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 21 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 21 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 21 | 0.14 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 21 | 0.14 |
| (1,960) | 1:A:6:ILE:HB | 1:B:106:ILE:HG21 | 20 | 0.14 |
| (1,960) | 1:A:6:ILE:HB | 1:B:106:ILE:HG22 | 20 | 0.14 |
| (1,960) | 1:A:6:ILE:HB | 1:B:106:ILE:HG23 | 20 | 0.14 |
| (1,812) | 1:A:70:VAL:H | 1:A:70:VAL:HB | 19 | 0.14 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB2 | 9 | 0.14 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB3 | 9 | 0.14 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB2 | 9 | 0.14 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB3 | 9 | 0.14 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB2 | 9 | 0.14 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB3 | 9 | 0.14 |
| (1,687) | 1:A:48:GLU:HA | 1:A:51:THR:HA | 22 | 0.14 |
| (1,637) | 1:A:45:ALA:HB1 | 1:A:46:TRP:HD1 | 9 | 0.14 |
| (1,637) | 1:A:45:ALA:HB2 | 1:A:46:TRP:HD1 | 9 | 0.14 |
| (1,637) | 1:A:45:ALA:HB3 | 1:A:46:TRP:HD1 | 9 | 0.14 |
| (1,547) | 1:A:35:LEU:H | 1:A:36:PHE:HA | 15 | 0.14 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 8 | 0.14 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 8 | 0.14 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 8 | 0.14 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 8 | 0.14 |
| (1,285) | 1:A:22:LEU:HA | 1:A:22:LEU:HG | 5 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 9 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 9 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 9 | 0.14 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 9 | 0.14 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 9 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 9 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 9 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 9 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 11 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 19 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 19 | 0.14 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 19 | 0.14 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 19 | 0.14 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 19 | 0.14 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 19 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 19 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 19 | 0.14 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 19 | 0.14 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 19 | 0.14 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 20 | 0.14 |
| (1,166) | 1:A:16:LEU:HB2 | 1:A:17:LYS:H | 20 | 0.14 |
| (1,166) | 1:A:16:LEU:HB3 | 1:A:17:LYS:H | 20 | 0.14 |
| (1,1530) | 1:B:132:LEU:HA | 1:B:132:LEU:HD11 | 7 | 0.14 |
| (1,1530) | 1:B:132:LEU:HA | 1:B:132:LEU:HD12 | 7 | 0.14 |
| (1,1530) | 1:B:132:LEU:HA | 1:B:132:LEU:HD13 | 7 | 0.14 |
| (1,1530) | 1:B:132:LEU:HA | 1:B:132:LEU:HD21 | 7 | 0.14 |
| (1,1530) | 1:B:132:LEU:HA | 1:B:132:LEU:HD22 | 7 | 0.14 |
| (1,1530) | 1:B:132:LEU:HA | 1:B:132:LEU:HD23 | 7 | 0.14 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 18 | 0.14 |
| (1,1507) | 1:B:131:ALA:HA | 1:B:116:LEU:HB2 | 5 | 0.14 |
| (1,1507) | 1:B:131:ALA:HA | 1:B:116:LEU:HB3 | 5 | 0.14 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 10 | 0.14 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 10 | 0.14 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 10 | 0.14 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 10 | 0.14 |
| (1,1415) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HA | 5 | 0.14 |
| (1,1415) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HA | 5 | 0.14 |
| (1,1415) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HA | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1415) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HA | 10 | 0.14 |
| (1,1415) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HA | 10 | 0.14 |
| (1,1415) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HA | 10 | 0.14 |
| (1,1339) | 1:B:122:LEU:HA | 1:B:122:LEU:HG | 4 | 0.14 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 11 | 0.14 |
| (1,1220) | 1:B:116:LEU:HB2 | 1:B:117:LYS:H | 11 | 0.14 |
| (1,1220) | 1:B:116:LEU:HB3 | 1:B:117:LYS:H | 11 | 0.14 |
| (1,1120) | 1:B:108:MET:HG2 | 1:B:106:ILE:HG12 | 2 | 0.14 |
| (1,1120) | 1:B:108:MET:HG2 | 1:B:106:ILE:HG13 | 2 | 0.14 |
| (1,1120) | 1:B:108:MET:HG3 | 1:B:106:ILE:HG12 | 2 | 0.14 |
| (1,1120) | 1:B:108:MET:HG3 | 1:B:106:ILE:HG13 | 2 | 0.14 |
| (1,1119) | 1:B:108:MET:HG2 | 1:B:106:ILE:HD11 | 3 | 0.14 |
| (1,1119) | 1:B:108:MET:HG2 | 1:B:106:ILE:HD12 | 3 | 0.14 |
| (1,1119) | 1:B:108:MET:HG2 | 1:B:106:ILE:HD13 | 3 | 0.14 |
| (1,1119) | 1:B:108:MET:HG3 | 1:B:106:ILE:HD11 | 3 | 0.14 |
| (1,1119) | 1:B:108:MET:HG3 | 1:B:106:ILE:HD12 | 3 | 0.14 |
| (1,1119) | 1:B:108:MET:HG3 | 1:B:106:ILE:HD13 | 3 | 0.14 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 1 | 0.13 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 2 | 0.13 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 2 | 0.13 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 2 | 0.13 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 2 | 0.13 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 2 | 0.13 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 2 | 0.13 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 2 | 0.13 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 2 | 0.13 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 2 | 0.13 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD1 | 16 | 0.13 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD2 | 16 | 0.13 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD1 | 16 | 0.13 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD2 | 16 | 0.13 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD1 | 16 | 0.13 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD2 | 16 | 0.13 |
| (1,968) | 1:A:8:MET:HE1 | 1:B:104:LEU:H | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,968) | 1:A:8:MET:HE2 | 1:B:104:LEU:H | 18 | 0.13 |
| (1,968) | 1:A:8:MET:HE3 | 1:B:104:LEU:H | 18 | 0.13 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB2 | 20 | 0.13 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB3 | 20 | 0.13 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB2 | 20 | 0.13 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB3 | 20 | 0.13 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB2 | 20 | 0.13 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB3 | 20 | 0.13 |
| (1,643) | 1:A:46:TRP:HB2 | 1:A:46:TRP:HH2 | 5 | 0.13 |
| (1,643) | 1:A:46:TRP:HB3 | 1:A:46:TRP:HH2 | 5 | 0.13 |
| (1,637) | 1:A:45:ALA:HB1 | 1:A:46:TRP:HD1 | 18 | 0.13 |
| (1,637) | 1:A:45:ALA:HB2 | 1:A:46:TRP:HD1 | 18 | 0.13 |
| (1,637) | 1:A:45:ALA:HB3 | 1:A:46:TRP:HD1 | 18 | 0.13 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 10 | 0.13 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 10 | 0.13 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 21 | 0.13 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 21 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 1 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 1 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 1 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 1 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 13 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 13 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 13 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 13 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 16 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 16 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 16 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 16 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 19 | 0.13 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 19 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 19 | 0.13 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 19 | 0.13 |
| (1,365) | 1:A:27:ILE:HG21 | 1:A:17:LYS:HA | 15 | 0.13 |
| (1,365) | 1:A:27:ILE:HG22 | 1:A:17:LYS:HA | 15 | 0.13 |
| (1,365) | 1:A:27:ILE:HG23 | 1:A:17:LYS:HA | 15 | 0.13 |
| (1,365) | 1:A:27:ILE:HG21 | 1:A:17:LYS:HA | 19 | 0.13 |
| (1,365) | 1:A:27:ILE:HG22 | 1:A:17:LYS:HA | 19 | 0.13 |
| (1,365) | 1:A:27:ILE:HG23 | 1:A:17:LYS:HA | 19 | 0.13 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG12 | 3 | 0.13 |
| (1,251) | 1:A:20:ALA:HB1 | 1:A:27:ILE:HG13 | 3 | 0.13 |
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG12 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,251) | 1:A:20:ALA:HB2 | 1:A:27:ILE:HG13 | 3 | 0.13 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG12 | 3 | 0.13 |
| (1,251) | 1:A:20:ALA:HB3 | 1:A:27:ILE:HG13 | 3 | 0.13 |
| (1,222) | 1:A:19:LEU:HA | 1:A:19:LEU:HG | 4 | 0.13 |
| (1,222) | 1:A:19:LEU:HA | 1:A:19:LEU:HG | 13 | 0.13 |
| (1,2079) | 1:B:131:ALA:HA | 1:A:35:LEU:H | 22 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 3 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 5 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 6 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 17 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 17 | 0.13 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 17 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 17 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 17 | 0.13 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 17 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 17 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 17 | 0.13 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG21 | 6 | 0.13 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG22 | 6 | 0.13 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG23 | 6 | 0.13 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 3 | 0.13 |
| (1,196) | 1:A:17:LYS:HD2 | 1:A:18:ALA:H | 15 | 0.13 |
| (1,196) | 1:A:17:LYS:HD3 | 1:A:18:ALA:H | 15 | 0.13 |
| (1,196) | 1:A:17:LYS:HD2 | 1:A:18:ALA:H | 23 | 0.13 |
| (1,196) | 1:A:17:LYS:HD3 | 1:A:18:ALA:H | 23 | 0.13 |
| (1,1753) | 1:B:149:LEU:HA | 1:B:152:MET:HB2 | 11 | 0.13 |
| (1,1753) | 1:B:149:LEU:HA | 1:B:152:MET:HB3 | 11 | 0.13 |
| (1,1741) | 1:B:148:GLU:HA | 1:B:151:THR:HA | 11 | 0.13 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB1 | 13 | 0.13 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB2 | 13 | 0.13 |
| (1,1649) | 1:B:141:ASP:H | 1:B:140:ALA:HB3 | 13 | 0.13 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 3 | 0.13 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 2 | 0.13 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 2 | 0.13 |
| (1,1601) | 1:B:135:LEU:H | 1:B:136:PHE:HA | 8 | 0.13 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 6 | 0.13 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 15 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 5 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 5 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 5 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 5 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 6 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 6 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 6 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 6 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 20 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 20 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 20 | 0.13 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 20 | 0.13 |
| (1,1315) | 1:B:120:ALA:HA | 1:B:131:ALA:H | 9 | 0.13 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 3 | 0.13 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 21 | 0.13 |
| (1,1204) | 1:B:114:GLN:H | 1:B:115:SER:HA | 10 | 0.13 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB2 | 12 | 0.13 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB3 | 12 | 0.13 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB2 | 12 | 0.13 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB3 | 12 | 0.13 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB2 | 12 | 0.13 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB3 | 12 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|------------------|----------|---------------|
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 9 | 0.12 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 9 | 0.12 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 9 | 0.12 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 9 | 0.12 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 9 | 0.12 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 9 | 0.12 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 9 | 0.12 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 9 | 0.12 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 9 | 0.12 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD1 | 15 | 0.12 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD2 | 15 | 0.12 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD1 | 15 | 0.12 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD2 | 15 | 0.12 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD1 | 15 | 0.12 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD2 | 15 | 0.12 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD1 | 22 | 0.12 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD2 | 22 | 0.12 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD1 | 22 | 0.12 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD2 | 22 | 0.12 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD1 | 22 | 0.12 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD2 | 22 | 0.12 |
| (1,861) | 1:A:77:GLU:H | 1:A:77:GLU:HA | 9 | 0.12 |
| (1,796) | 1:A:67:THR:H | 1:A:67:THR:HA | 3 | 0.12 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB2 | 4 | 0.12 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB3 | 4 | 0.12 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB2 | 4 | 0.12 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB3 | 4 | 0.12 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB2 | 4 | 0.12 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB3 | 4 | 0.12 |
| (1,610) | 1:A:43:ASP:H | 1:A:43:ASP:HA | 12 | 0.12 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB1 | 8 | 0.12 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB2 | 8 | 0.12 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB3 | 8 | 0.12 |
| (1,587) | 1:A:40:ALA:H | 1:A:39:ASP:HA | 6 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 1 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 1 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 3 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 3 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 4 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 4 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 5 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 5 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 6 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 6 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 7 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 7 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 8 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 8 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 9 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 9 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 11 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 11 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 12 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 12 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 13 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 13 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 14 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 14 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 15 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 15 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 16 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 16 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 17 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 17 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 18 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 18 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 19 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 19 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 20 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 20 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 22 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 22 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 23 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 23 | 0.12 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 24 | 0.12 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 24 | 0.12 |
| (1,547) | 1:A:35:LEU:H | 1:A:36:PHE:HA | 13 | 0.12 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 24 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 2 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 2 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 2 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 2 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 3 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 3 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 3 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 3 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 6 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 6 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 6 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 6 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 12 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 12 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 12 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 12 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 20 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 20 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 20 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 20 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 21 | 0.12 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 21 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 21 | 0.12 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 21 | 0.12 |
| (1,281) | 1:A:22:LEU:HB2 | 1:A:21:ALA:H | 15 | 0.12 |
| (1,281) | 1:A:22:LEU:HB3 | 1:A:21:ALA:H | 15 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 8 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 10 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 13 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 13 | 0.12 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 13 | 0.12 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 13 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 13 | 0.12 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 13 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 13 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 13 | 0.12 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 13 | 0.12 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD1 | 11 | 0.12 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD2 | 11 | 0.12 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD1 | 11 | 0.12 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD2 | 11 | 0.12 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD1 | 11 | 0.12 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD2 | 11 | 0.12 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD1 | 15 | 0.12 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD2 | 15 | 0.12 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD1 | 15 | 0.12 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD2 | 15 | 0.12 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD1 | 15 | 0.12 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD2 | 15 | 0.12 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 18 | 0.12 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 21 | 0.12 |
| (1,2006) | 1:B:106:ILE:HD11 | 1:A:4:LEU:H | 23 | 0.12 |
| (1,2006) | 1:B:106:ILE:HD12 | 1:A:4:LEU:H | 23 | 0.12 |
| (1,2006) | 1:B:106:ILE:HD13 | 1:A:4:LEU:H | 23 | 0.12 |
| (1,183) | 1:A:17:LYS:HE2 | 1:A:13:HIS:HD2 | 23 | 0.12 |
| (1,183) | 1:A:17:LYS:HE3 | 1:A:13:HIS:HD2 | 23 | 0.12 |
| (1,1818) | 1:B:161:LEU:H | 1:B:161:LEU:HA | 3 | 0.12 |
| (1,1691) | 1:B:145:ALA:HB1 | 1:B:146:TRP:HD1 | 17 | 0.12 |
| (1,1691) | 1:B:145:ALA:HB2 | 1:B:146:TRP:HD1 | 17 | 0.12 |
| (1,1691) | 1:B:145:ALA:HB3 | 1:B:146:TRP:HD1 | 17 | 0.12 |
| (1,1665) | 1:B:143:ASP:H | 1:B:143:ASP:HB2 | 3 | 0.12 |
| (1,1665) | 1:B:143:ASP:H | 1:B:143:ASP:HB3 | 3 | 0.12 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 11 | 0.12 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 18 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 1 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 1 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 3 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 3 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 5 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 5 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 6 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 6 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 7 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 7 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 8 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 8 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 9 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 9 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 11 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 11 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 12 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 12 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 13 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 13 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 14 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 14 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 15 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 15 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 16 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 16 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 17 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 17 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 18 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 18 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 19 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 19 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 20 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 20 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 21 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 21 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 22 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 22 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 24 | 0.12 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 24 | 0.12 |
| (1,1601) | 1:B:135:LEU:H | 1:B:136:PHE:HA | 13 | 0.12 |
| (1,1583) | 1:B:134:ARG:H | 1:B:133:GLU:HA | 23 | 0.12 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 14 | 0.12 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 20 | 0.12 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 21 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 1 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 1 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 1 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 1 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 2 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 2 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 2 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 12 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 12 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 12 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 12 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 13 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 13 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 13 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 13 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 15 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 15 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 15 | 0.12 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 15 | 0.12 |
| (1,1419) | 1:B:127:ILE:HG21 | 1:B:117:LYS:HA | 11 | 0.12 |
| (1,1419) | 1:B:127:ILE:HG22 | 1:B:117:LYS:HA | 11 | 0.12 |
| (1,1419) | 1:B:127:ILE:HG23 | 1:B:117:LYS:HA | 11 | 0.12 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 6 | 0.12 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 15 | 0.12 |
| (1,1220) | 1:B:116:LEU:HB2 | 1:B:117:LYS:H | 23 | 0.12 |
| (1,1220) | 1:B:116:LEU:HB3 | 1:B:117:LYS:H | 23 | 0.12 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB2 | 6 | 0.12 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB3 | 6 | 0.12 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB2 | 6 | 0.12 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB3 | 6 | 0.12 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB2 | 6 | 0.12 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB3 | 6 | 0.12 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB2 | 18 | 0.12 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB3 | 18 | 0.12 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB2 | 18 | 0.12 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB3 | 18 | 0.12 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB2 | 18 | 0.12 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB3 | 18 | 0.12 |
| (1,1118) | 1:B:108:MET:HG2 | 1:B:106:ILE:HA | 17 | 0.12 |
| (1,1118) | 1:B:108:MET:HG3 | 1:B:106:ILE:HA | 17 | 0.12 |
| (1,1025) | 1:A:31:ALA:HA | 1:B:135:LEU:H | 2 | 0.12 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD11 | 24 | 0.11 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD12 | 24 | 0.11 |
| (1,984) | 1:A:8:MET:HE1 | 1:B:127:ILE:HD13 | 24 | 0.11 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD11 | 24 | 0.11 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD12 | 24 | 0.11 |
| (1,984) | 1:A:8:MET:HE2 | 1:B:127:ILE:HD13 | 24 | 0.11 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD11 | 24 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|------------------|----------|---------------|
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD12 | 24 | 0.11 |
| (1,984) | 1:A:8:MET:HE3 | 1:B:127:ILE:HD13 | 24 | 0.11 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD1 | 19 | 0.11 |
| (1,971) | 1:A:8:MET:HE1 | 1:B:136:PHE:HD2 | 19 | 0.11 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD1 | 19 | 0.11 |
| (1,971) | 1:A:8:MET:HE2 | 1:B:136:PHE:HD2 | 19 | 0.11 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD1 | 19 | 0.11 |
| (1,971) | 1:A:8:MET:HE3 | 1:B:136:PHE:HD2 | 19 | 0.11 |
| (1,779) | 1:A:64:LYS:HE2 | 1:A:64:LYS:HB2 | 19 | 0.11 |
| (1,779) | 1:A:64:LYS:HE2 | 1:A:64:LYS:HB3 | 19 | 0.11 |
| (1,779) | 1:A:64:LYS:HE3 | 1:A:64:LYS:HB2 | 19 | 0.11 |
| (1,779) | 1:A:64:LYS:HE3 | 1:A:64:LYS:HB3 | 19 | 0.11 |
| (1,769) | 1:A:62:ALA:H | 1:A:62:ALA:HA | 18 | 0.11 |
| (1,751) | 1:A:58:ASN:H | 1:A:58:ASN:HA | 5 | 0.11 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB2 | 3 | 0.11 |
| (1,69) | 1:A:8:MET:HE1 | 1:A:8:MET:HB3 | 3 | 0.11 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB2 | 3 | 0.11 |
| (1,69) | 1:A:8:MET:HE2 | 1:A:8:MET:HB3 | 3 | 0.11 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB2 | 3 | 0.11 |
| (1,69) | 1:A:8:MET:HE3 | 1:A:8:MET:HB3 | 3 | 0.11 |
| (1,65) | 1:A:8:MET:HG2 | 1:A:6:ILE:HD11 | 3 | 0.11 |
| (1,65) | 1:A:8:MET:HG2 | 1:A:6:ILE:HD12 | 3 | 0.11 |
| (1,65) | 1:A:8:MET:HG2 | 1:A:6:ILE:HD13 | 3 | 0.11 |
| (1,65) | 1:A:8:MET:HG3 | 1:A:6:ILE:HD11 | 3 | 0.11 |
| (1,65) | 1:A:8:MET:HG3 | 1:A:6:ILE:HD12 | 3 | 0.11 |
| (1,65) | 1:A:8:MET:HG3 | 1:A:6:ILE:HD13 | 3 | 0.11 |
| (1,610) | 1:A:43:ASP:H | 1:A:43:ASP:HA | 17 | 0.11 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB1 | 15 | 0.11 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB2 | 15 | 0.11 |
| (1,595) | 1:A:41:ASP:H | 1:A:40:ALA:HB3 | 15 | 0.11 |
| (1,589) | 1:A:40:ALA:H | 1:A:40:ALA:HA | 1 | 0.11 |
| (1,589) | 1:A:40:ALA:H | 1:A:40:ALA:HA | 19 | 0.11 |
| (1,589) | 1:A:40:ALA:H | 1:A:40:ALA:HA | 22 | 0.11 |
| (1,589) | 1:A:40:ALA:H | 1:A:40:ALA:HA | 24 | 0.11 |
| (1,553) | 1:A:36:PHE:HB2 | 1:A:36:PHE:HZ | 2 | 0.11 |
| (1,553) | 1:A:36:PHE:HB3 | 1:A:36:PHE:HZ | 2 | 0.11 |
| (1,518) | 1:A:34:ARG:HA | 1:A:36:PHE:HB2 | 16 | 0.11 |
| (1,518) | 1:A:34:ARG:HA | 1:A:36:PHE:HB3 | 16 | 0.11 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 3 | 0.11 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 5 | 0.11 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 7 | 0.11 |
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 12 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,474) | 1:A:32:LEU:HA | 1:A:31:ALA:H | 14 | 0.11 |
| (1,463) | 1:A:31:ALA:HA | 1:A:32:LEU:HB2 | 11 | 0.11 |
| (1,463) | 1:A:31:ALA:HA | 1:A:32:LEU:HB3 | 11 | 0.11 |
| (1,453) | 1:A:31:ALA:HA | 1:A:16:LEU:HB2 | 23 | 0.11 |
| (1,453) | 1:A:31:ALA:HA | 1:A:16:LEU:HB3 | 23 | 0.11 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 11 | 0.11 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 11 | 0.11 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 11 | 0.11 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 11 | 0.11 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD1 | 23 | 0.11 |
| (1,420) | 1:A:29:GLN:HB2 | 1:A:30:TYR:HD2 | 23 | 0.11 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD1 | 23 | 0.11 |
| (1,420) | 1:A:29:GLN:HB3 | 1:A:30:TYR:HD2 | 23 | 0.11 |
| (1,362) | 1:A:27:ILE:HD11 | 1:A:17:LYS:HG2 | 19 | 0.11 |
| (1,362) | 1:A:27:ILE:HD11 | 1:A:17:LYS:HG3 | 19 | 0.11 |
| (1,362) | 1:A:27:ILE:HD12 | 1:A:17:LYS:HG2 | 19 | 0.11 |
| (1,362) | 1:A:27:ILE:HD12 | 1:A:17:LYS:HG3 | 19 | 0.11 |
| (1,362) | 1:A:27:ILE:HD13 | 1:A:17:LYS:HG2 | 19 | 0.11 |
| (1,362) | 1:A:27:ILE:HD13 | 1:A:17:LYS:HG3 | 19 | 0.11 |
| (1,261) | 1:A:20:ALA:HA | 1:A:31:ALA:H | 10 | 0.11 |
| (1,2079) | 1:B:131:ALA:HA | 1:A:35:LEU:H | 10 | 0.11 |
| (1,2079) | 1:B:131:ALA:HA | 1:A:35:LEU:H | 18 | 0.11 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD11 | 16 | 0.11 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD12 | 16 | 0.11 |
| (1,2038) | 1:B:108:MET:HE1 | 1:A:27:ILE:HD13 | 16 | 0.11 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD11 | 16 | 0.11 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD12 | 16 | 0.11 |
| (1,2038) | 1:B:108:MET:HE2 | 1:A:27:ILE:HD13 | 16 | 0.11 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD11 | 16 | 0.11 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD12 | 16 | 0.11 |
| (1,2038) | 1:B:108:MET:HE3 | 1:A:27:ILE:HD13 | 16 | 0.11 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD1 | 13 | 0.11 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD2 | 13 | 0.11 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD1 | 13 | 0.11 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD2 | 13 | 0.11 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD1 | 13 | 0.11 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD2 | 13 | 0.11 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD1 | 20 | 0.11 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD2 | 20 | 0.11 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD1 | 20 | 0.11 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD2 | 20 | 0.11 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD1 | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD2 | 20 | 0.11 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD1 | 24 | 0.11 |
| (1,2025) | 1:B:108:MET:HE1 | 1:A:36:PHE:HD2 | 24 | 0.11 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD1 | 24 | 0.11 |
| (1,2025) | 1:B:108:MET:HE2 | 1:A:36:PHE:HD2 | 24 | 0.11 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD1 | 24 | 0.11 |
| (1,2025) | 1:B:108:MET:HE3 | 1:A:36:PHE:HD2 | 24 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG21 | 2 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG22 | 2 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG23 | 2 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG21 | 4 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG22 | 4 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG23 | 4 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG21 | 13 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG22 | 13 | 0.11 |
| (1,2014) | 1:B:106:ILE:HB | 1:A:6:ILE:HG23 | 13 | 0.11 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 2 | 0.11 |
| (1,201) | 1:A:17:LYS:H | 1:A:14:GLN:H | 24 | 0.11 |
| (1,1973) | 1:B:104:LEU:HG | 1:A:5:THR:HG21 | 18 | 0.11 |
| (1,1973) | 1:B:104:LEU:HG | 1:A:5:THR:HG22 | 18 | 0.11 |
| (1,1973) | 1:B:104:LEU:HG | 1:A:5:THR:HG23 | 18 | 0.11 |
| (1,1907) | 1:B:176:GLU:H | 1:B:176:GLU:HA | 14 | 0.11 |
| (1,180) | 1:A:16:LEU:H | 1:A:19:LEU:HB2 | 4 | 0.11 |
| (1,180) | 1:A:16:LEU:H | 1:A:19:LEU:HB3 | 4 | 0.11 |
| (1,180) | 1:A:16:LEU:H | 1:A:19:LEU:HB2 | 15 | 0.11 |
| (1,180) | 1:A:16:LEU:H | 1:A:19:LEU:HB3 | 15 | 0.11 |
| (1,1728) | 1:B:147:GLN:H | 1:B:146:TRP:HA | 5 | 0.11 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 7 | 0.11 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 8 | 0.11 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 16 | 0.11 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 21 | 0.11 |
| (1,1643) | 1:B:140:ALA:H | 1:B:140:ALA:HA | 24 | 0.11 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 4 | 0.11 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 4 | 0.11 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 10 | 0.11 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 10 | 0.11 |
| (1,1607) | 1:B:136:PHE:HB2 | 1:B:136:PHE:HZ | 23 | 0.11 |
| (1,1607) | 1:B:136:PHE:HB3 | 1:B:136:PHE:HZ | 23 | 0.11 |
| (1,1583) | 1:B:134:ARG:H | 1:B:133:GLU:HA | 13 | 0.11 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 2 | 0.11 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 10 | 0.11 |
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 17 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1528) | 1:B:132:LEU:HA | 1:B:131:ALA:H | 24 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 4 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 4 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 4 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 4 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 18 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 18 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 18 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 18 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 19 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 19 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 19 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 19 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD1 | 22 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB2 | 1:B:130:TYR:HD2 | 22 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD1 | 22 | 0.11 |
| (1,1474) | 1:B:129:GLN:HB3 | 1:B:130:TYR:HD2 | 22 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG21 | 1:B:117:LYS:HA | 10 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG22 | 1:B:117:LYS:HA | 10 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG23 | 1:B:117:LYS:HA | 10 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG21 | 1:B:117:LYS:HA | 23 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG22 | 1:B:117:LYS:HA | 23 | 0.11 |
| (1,1419) | 1:B:127:ILE:HG23 | 1:B:117:LYS:HA | 23 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HG2 | 10 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HG3 | 10 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HG2 | 10 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HG3 | 10 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HG2 | 10 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HG3 | 10 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HG2 | 12 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD11 | 1:B:117:LYS:HG3 | 12 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HG2 | 12 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD12 | 1:B:117:LYS:HG3 | 12 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HG2 | 12 | 0.11 |
| (1,1416) | 1:B:127:ILE:HD13 | 1:B:117:LYS:HG3 | 12 | 0.11 |
| (1,1315) | 1:B:120:ALA:HA | 1:B:131:ALA:H | 11 | 0.11 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 12 | 0.11 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 13 | 0.11 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 19 | 0.11 |
| (1,1255) | 1:B:117:LYS:H | 1:B:114:GLN:H | 20 | 0.11 |
| (1,1236) | 1:B:117:LYS:HD2 | 1:B:113:HIS:HD2 | 5 | 0.11 |
| (1,1236) | 1:B:117:LYS:HD3 | 1:B:113:HIS:HD2 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|------------|-----------------|------------------|-----------------|----------------------|
| (1,1234) | 1:B:116:LEU:H | 1:B:119:LEU:HB2 | 17 | 0.11 |
| (1,1234) | 1:B:116:LEU:H | 1:B:119:LEU:HB3 | 17 | 0.11 |
| (1,1204) | 1:B:114:GLN:H | 1:B:115:SER:HA | 2 | 0.11 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB2 | 16 | 0.11 |
| (1,1123) | 1:B:108:MET:HE1 | 1:B:108:MET:HB3 | 16 | 0.11 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB2 | 16 | 0.11 |
| (1,1123) | 1:B:108:MET:HE2 | 1:B:108:MET:HB3 | 16 | 0.11 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB2 | 16 | 0.11 |
| (1,1123) | 1:B:108:MET:HE3 | 1:B:108:MET:HB3 | 16 | 0.11 |
| (1,1120) | 1:B:108:MET:HG2 | 1:B:106:ILE:HG12 | 6 | 0.11 |
| (1,1120) | 1:B:108:MET:HG2 | 1:B:106:ILE:HG13 | 6 | 0.11 |
| (1,1120) | 1:B:108:MET:HG3 | 1:B:106:ILE:HG12 | 6 | 0.11 |
| (1,1120) | 1:B:108:MET:HG3 | 1:B:106:ILE:HG13 | 6 | 0.11 |
| (1,1025) | 1:A:31:ALA:HA | 1:B:135:LEU:H | 17 | 0.11 |

10 Dihedral-angle violation analysis

No dihedral-angle restraints found