



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 01:03 PM EST

PDB ID : 6NOM
BMRB ID : 30561
Title : NMR solution structure of Pisum sativum defensin 2 (Psd2) provides evidence for the presence of hydrophobic surface clusters
Authors : Pinheiro-Aguiar, R.; Amaral, V.S.G.; Bastos, I.; Kurtenbach, E.; Almeida, F.C.L.
Deposited on : 2019-01-16

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

We welcome your comments at validation@mail.wwpdb.org

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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

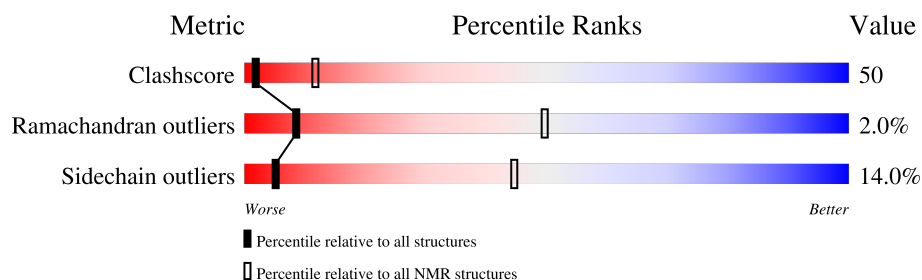
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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 | 210492 | 14027 |
| Ramachandran outliers | 207382 | 12486 |
| Sidechain outliers | 206894 | 12463 |

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 | 47 | <div> <div>43%</div> <div>51%</div> <div>6%</div> </div> |

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:1-A:47 (47) | 0.55 | 13 |

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 5 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 715 atoms, of which 343 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Defensin-2.

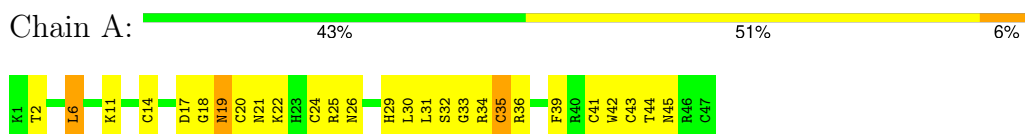
| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1 | A | 47 | Total | C | H | N | O | S | 0 |
| | | | 715 | 219 | 343 | 76 | 69 | 8 | |

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: Defensin-2

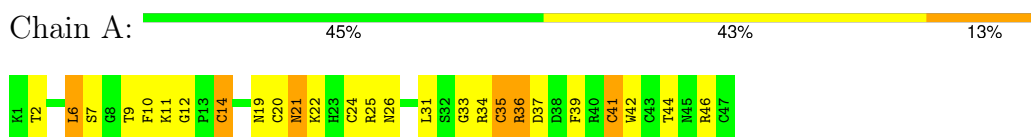


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

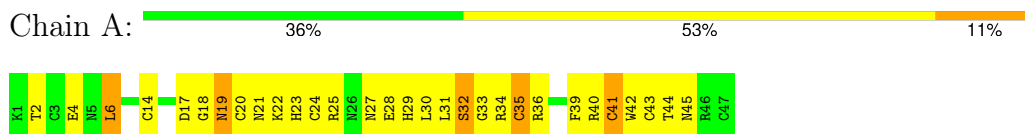
4.2.1 Score per residue for model 1

- Molecule 1: Defensin-2



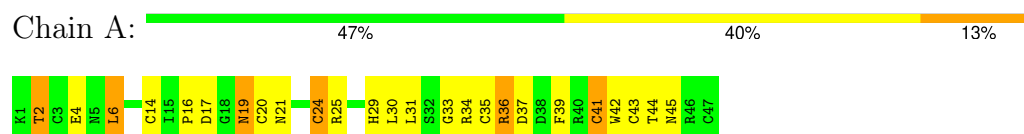
4.2.2 Score per residue for model 2

- Molecule 1: Defensin-2



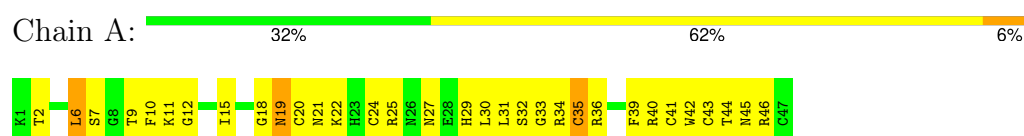
4.2.3 Score per residue for model 3

- Molecule 1: Defensin-2



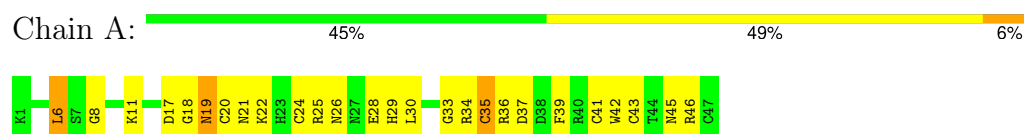
4.2.4 Score per residue for model 4

- Molecule 1: Defensin-2



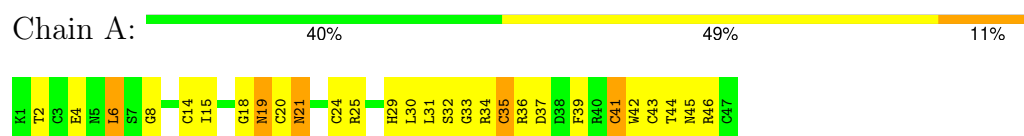
4.2.5 Score per residue for model 5

- Molecule 1: Defensin-2



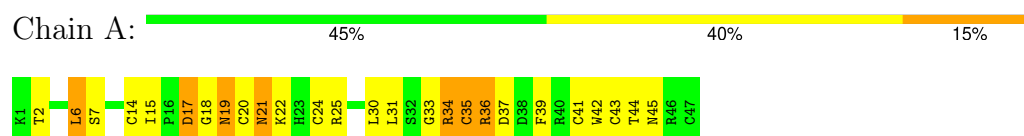
4.2.6 Score per residue for model 6

- Molecule 1: Defensin-2



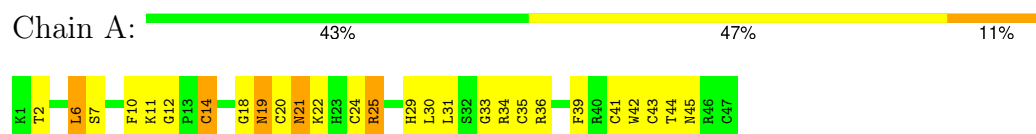
4.2.7 Score per residue for model 7

- Molecule 1: Defensin-2



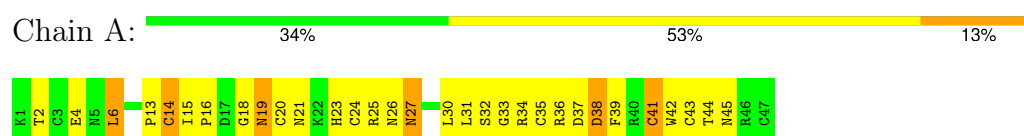
4.2.8 Score per residue for model 8

- Molecule 1: Defensin-2



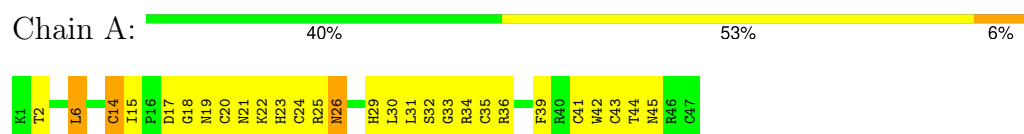
4.2.9 Score per residue for model 9

- Molecule 1: Defensin-2



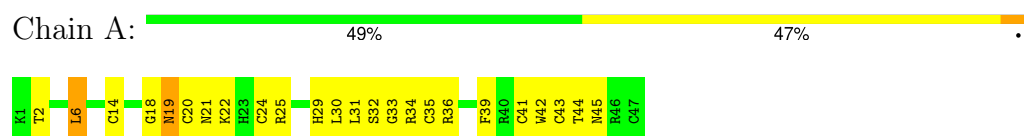
4.2.10 Score per residue for model 10

- Molecule 1: Defensin-2



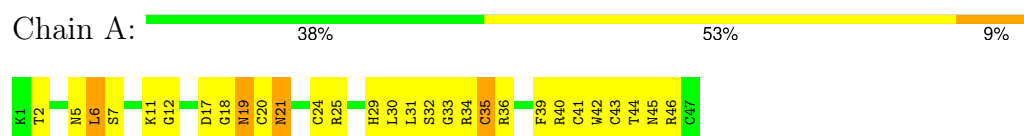
4.2.11 Score per residue for model 11

- Molecule 1: Defensin-2



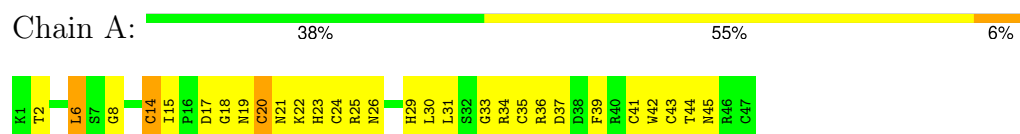
4.2.12 Score per residue for model 12

- Molecule 1: Defensin-2



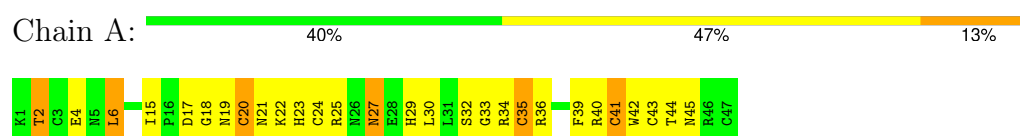
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Defensin-2



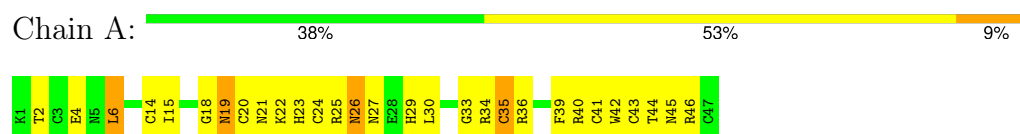
4.2.14 Score per residue for model 14

- Molecule 1: Defensin-2



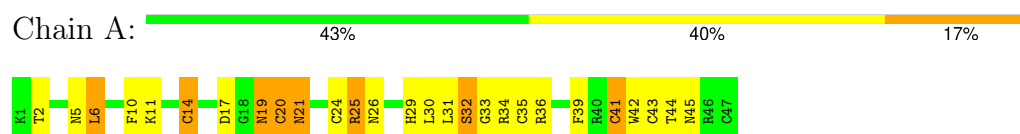
4.2.15 Score per residue for model 15

- Molecule 1: Defensin-2



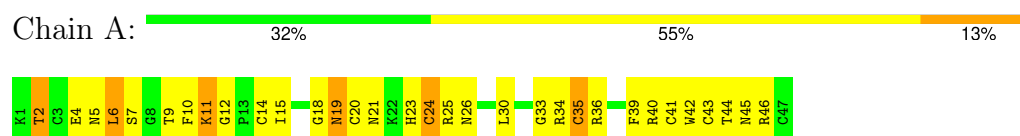
4.2.16 Score per residue for model 16

- Molecule 1: Defensin-2



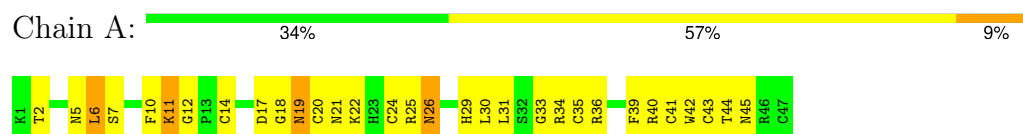
4.2.17 Score per residue for model 17

- Molecule 1: Defensin-2



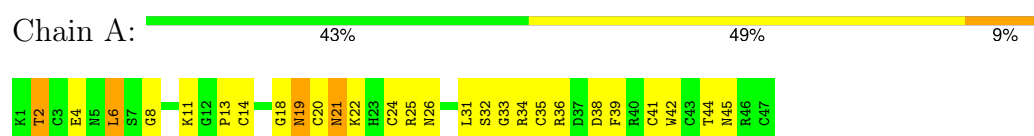
4.2.18 Score per residue for model 18

- Molecule 1: Defensin-2



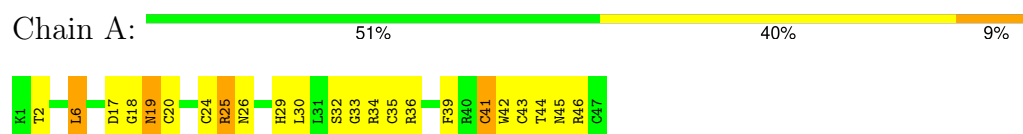
4.2.19 Score per residue for model 19

- Molecule 1: Defensin-2



4.2.20 Score per residue for model 20

- Molecule 1: Defensin-2



5 Refinement protocol and experimental data overview

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

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

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| CNS | refinement | |
| ARIA | structure calculation | |

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

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 489 |
| Number of shifts mapped to atoms | 489 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 80% |

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 | 372 | 343 | 341 | 35±3 |
| All | All | 7440 | 6860 | 6820 | 706 |

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 50.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:30:LEU:HD12 | 1:A:43:CYS:SG | 0.84 | 2.11 | 9 | 15 |
| 1:A:33:GLY:HA2 | 1:A:43:CYS:SG | 0.84 | 2.12 | 3 | 16 |
| 1:A:21:ASN:HA | 1:A:33:GLY:O | 0.81 | 1.75 | 18 | 18 |
| 1:A:20:CYS:HA | 1:A:35:CYS:O | 0.81 | 1.76 | 17 | 20 |
| 1:A:34:ARG:HB3 | 1:A:41:CYS:SG | 0.80 | 2.16 | 14 | 7 |
| 1:A:34:ARG:HB2 | 1:A:42:TRP:O | 0.78 | 1.77 | 12 | 13 |
| 1:A:30:LEU:HD22 | 1:A:43:CYS:SG | 0.78 | 2.18 | 5 | 2 |
| 1:A:34:ARG:HG2 | 1:A:41:CYS:SG | 0.72 | 2.23 | 20 | 13 |
| 1:A:34:ARG:CB | 1:A:41:CYS:HB3 | 0.71 | 2.15 | 8 | 19 |
| 1:A:24:CYS:CB | 1:A:33:GLY:HA2 | 0.70 | 2.17 | 4 | 20 |
| 1:A:34:ARG:HB3 | 1:A:41:CYS:CB | 0.68 | 2.18 | 9 | 9 |
| 1:A:18:GLY:H | 1:A:36:ARG:CZ | 0.68 | 2.02 | 7 | 2 |
| 1:A:25:ARG:CD | 1:A:33:GLY:HA3 | 0.68 | 2.18 | 8 | 3 |
| 1:A:24:CYS:SG | 1:A:35:CYS:HB2 | 0.68 | 2.29 | 11 | 10 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:34:ARG:HB3 | 1:A:42:TRP:N | 0.67 | 2.05 | 7 | 13 |
| 1:A:20:CYS:HB3 | 1:A:36:ARG:CG | 0.66 | 2.20 | 13 | 8 |
| 1:A:34:ARG:HB3 | 1:A:41:CYS:HB3 | 0.65 | 1.68 | 13 | 20 |
| 1:A:34:ARG:HD3 | 1:A:42:TRP:N | 0.65 | 2.06 | 3 | 3 |
| 1:A:24:CYS:HB3 | 1:A:33:GLY:HA2 | 0.64 | 1.69 | 17 | 10 |
| 1:A:6:LEU:HD23 | 1:A:41:CYS:O | 0.64 | 1.92 | 19 | 17 |
| 1:A:30:LEU:HD22 | 1:A:45:ASN:ND2 | 0.63 | 2.09 | 17 | 16 |
| 1:A:20:CYS:HB2 | 1:A:35:CYS:N | 0.62 | 2.10 | 7 | 13 |
| 1:A:4:GLU:HB2 | 1:A:44:THR:HG23 | 0.61 | 1.71 | 2 | 8 |
| 1:A:2:THR:HB | 1:A:45:ASN:O | 0.61 | 1.94 | 3 | 4 |
| 1:A:19:ASN:HD22 | 1:A:19:ASN:H | 0.61 | 1.39 | 18 | 7 |
| 1:A:19:ASN:ND2 | 1:A:19:ASN:H | 0.59 | 1.94 | 6 | 10 |
| 1:A:19:ASN:HD22 | 1:A:19:ASN:N | 0.58 | 1.96 | 9 | 7 |
| 1:A:17:ASP:HB2 | 1:A:19:ASN:ND2 | 0.58 | 2.13 | 16 | 8 |
| 1:A:24:CYS:HB3 | 1:A:33:GLY:CA | 0.58 | 2.27 | 3 | 2 |
| 1:A:34:ARG:HD3 | 1:A:42:TRP:H | 0.58 | 1.57 | 3 | 13 |
| 1:A:5:ASN:HD21 | 1:A:11:LYS:CB | 0.58 | 2.12 | 18 | 2 |
| 1:A:2:THR:OG1 | 1:A:31:LEU:HD12 | 0.57 | 1.98 | 4 | 13 |
| 1:A:34:ARG:HB2 | 1:A:42:TRP:N | 0.57 | 2.14 | 2 | 6 |
| 1:A:6:LEU:HD21 | 1:A:41:CYS:N | 0.57 | 2.15 | 3 | 3 |
| 1:A:2:THR:OG1 | 1:A:44:THR:HG22 | 0.57 | 1.98 | 7 | 11 |
| 1:A:15:ILE:HB | 1:A:17:ASP:OD1 | 0.57 | 1.99 | 7 | 1 |
| 1:A:20:CYS:HB2 | 1:A:34:ARG:C | 0.57 | 2.19 | 3 | 14 |
| 1:A:34:ARG:O | 1:A:41:CYS:HB3 | 0.57 | 2.00 | 6 | 2 |
| 1:A:28:GLU:HB3 | 1:A:30:LEU:CD1 | 0.57 | 2.30 | 5 | 2 |
| 1:A:20:CYS:HB3 | 1:A:36:ARG:HG3 | 0.57 | 1.75 | 13 | 6 |
| 1:A:18:GLY:HA2 | 1:A:36:ARG:NE | 0.57 | 2.14 | 15 | 3 |
| 1:A:36:ARG:CD | 1:A:39:PHE:HB2 | 0.56 | 2.30 | 19 | 8 |
| 1:A:20:CYS:HB3 | 1:A:36:ARG:CD | 0.56 | 2.30 | 7 | 6 |
| 1:A:20:CYS:HB2 | 1:A:34:ARG:CA | 0.56 | 2.30 | 3 | 1 |
| 1:A:36:ARG:HD2 | 1:A:39:PHE:CB | 0.56 | 2.31 | 1 | 1 |
| 1:A:22:LYS:O | 1:A:26:ASN:HB2 | 0.56 | 2.01 | 18 | 3 |
| 1:A:30:LEU:HD12 | 1:A:30:LEU:N | 0.55 | 2.16 | 2 | 2 |
| 1:A:7:SER:HA | 1:A:12:GLY:O | 0.55 | 2.01 | 4 | 6 |
| 1:A:30:LEU:HG | 1:A:45:ASN:ND2 | 0.54 | 2.18 | 2 | 1 |
| 1:A:11:LYS:N | 1:A:11:LYS:HD2 | 0.54 | 2.17 | 5 | 1 |
| 1:A:25:ARG:HA | 1:A:29:HIS:HA | 0.54 | 1.80 | 16 | 3 |
| 1:A:32:SER:HB2 | 1:A:44:THR:OG1 | 0.54 | 2.02 | 4 | 11 |
| 1:A:14:CYS:SG | 1:A:15:ILE:HG12 | 0.54 | 2.43 | 6 | 2 |
| 1:A:24:CYS:HB2 | 1:A:33:GLY:HA2 | 0.53 | 1.80 | 10 | 2 |
| 1:A:34:ARG:HB2 | 1:A:42:TRP:C | 0.53 | 2.23 | 13 | 7 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:34:ARG:HB3 | 1:A:41:CYS:C | 0.53 | 2.24 | 5 | 12 |
| 1:A:36:ARG:HD2 | 1:A:39:PHE:HB2 | 0.53 | 1.80 | 1 | 11 |
| 1:A:19:ASN:CB | 1:A:22:LYS:HE2 | 0.53 | 2.34 | 19 | 4 |
| 1:A:34:ARG:C | 1:A:41:CYS:HB3 | 0.53 | 2.23 | 1 | 13 |
| 1:A:14:CYS:HB3 | 1:A:36:ARG:O | 0.53 | 2.03 | 11 | 4 |
| 1:A:25:ARG:HD3 | 1:A:33:GLY:HA3 | 0.53 | 1.80 | 16 | 12 |
| 1:A:31:LEU:N | 1:A:31:LEU:HD12 | 0.53 | 2.19 | 10 | 2 |
| 1:A:20:CYS:HB3 | 1:A:36:ARG:HG2 | 0.52 | 1.81 | 7 | 3 |
| 1:A:24:CYS:HB2 | 1:A:33:GLY:CA | 0.52 | 2.33 | 1 | 6 |
| 1:A:15:ILE:HG13 | 1:A:36:ARG:NH2 | 0.52 | 2.19 | 9 | 2 |
| 1:A:20:CYS:SG | 1:A:34:ARG:HG2 | 0.52 | 2.45 | 7 | 2 |
| 1:A:34:ARG:HD2 | 1:A:42:TRP:H | 0.52 | 1.65 | 14 | 5 |
| 1:A:36:ARG:HB2 | 1:A:39:PHE:O | 0.52 | 2.05 | 7 | 2 |
| 1:A:16:PRO:HA | 1:A:38:ASP:OD1 | 0.52 | 2.05 | 9 | 1 |
| 1:A:36:ARG:HG3 | 1:A:39:PHE:O | 0.51 | 2.06 | 6 | 6 |
| 1:A:36:ARG:NE | 1:A:39:PHE:HB2 | 0.51 | 2.20 | 15 | 3 |
| 1:A:15:ILE:HD11 | 1:A:35:CYS:O | 0.51 | 2.06 | 9 | 1 |
| 1:A:34:ARG:HD2 | 1:A:42:TRP:N | 0.50 | 2.21 | 14 | 2 |
| 1:A:18:GLY:HA2 | 1:A:36:ARG:HD2 | 0.50 | 1.82 | 20 | 10 |
| 1:A:24:CYS:HB2 | 1:A:33:GLY:O | 0.50 | 2.07 | 14 | 6 |
| 1:A:18:GLY:H | 1:A:36:ARG:NH2 | 0.49 | 2.03 | 9 | 1 |
| 1:A:6:LEU:HD23 | 1:A:41:CYS:C | 0.49 | 2.28 | 2 | 7 |
| 1:A:15:ILE:HD12 | 1:A:19:ASN:ND2 | 0.49 | 2.23 | 7 | 1 |
| 1:A:36:ARG:CG | 1:A:41:CYS:HB2 | 0.49 | 2.38 | 9 | 1 |
| 1:A:5:ASN:HD21 | 1:A:11:LYS:HB3 | 0.49 | 1.67 | 12 | 1 |
| 1:A:21:ASN:O | 1:A:25:ARG:HG2 | 0.48 | 2.08 | 11 | 6 |
| 1:A:33:GLY:CA | 1:A:43:CYS:SG | 0.48 | 3.01 | 17 | 5 |
| 1:A:36:ARG:HD3 | 1:A:39:PHE:HB2 | 0.48 | 1.85 | 11 | 4 |
| 1:A:20:CYS:CB | 1:A:36:ARG:HG2 | 0.48 | 2.38 | 9 | 1 |
| 1:A:18:GLY:H | 1:A:36:ARG:NH1 | 0.48 | 2.06 | 7 | 1 |
| 1:A:22:LYS:HB2 | 1:A:26:ASN:OD1 | 0.48 | 2.09 | 5 | 1 |
| 1:A:36:ARG:HG2 | 1:A:41:CYS:HB2 | 0.48 | 1.86 | 8 | 5 |
| 1:A:20:CYS:HB3 | 1:A:36:ARG:HD3 | 0.48 | 1.86 | 3 | 1 |
| 1:A:15:ILE:HG12 | 1:A:35:CYS:SG | 0.48 | 2.49 | 9 | 2 |
| 1:A:19:ASN:ND2 | 1:A:19:ASN:N | 0.48 | 2.60 | 6 | 6 |
| 1:A:21:ASN:HD22 | 1:A:21:ASN:N | 0.47 | 2.07 | 16 | 1 |
| 1:A:36:ARG:NH1 | 1:A:36:ARG:HB3 | 0.47 | 2.25 | 7 | 1 |
| 1:A:2:THR:OG1 | 1:A:31:LEU:HD22 | 0.47 | 2.09 | 11 | 1 |
| 1:A:30:LEU:HD23 | 1:A:45:ASN:HB2 | 0.47 | 1.86 | 5 | 2 |
| 1:A:8:GLY:HA2 | 1:A:37:ASP:HA | 0.47 | 1.86 | 13 | 2 |
| 1:A:19:ASN:OD1 | 1:A:23:HIS:HB2 | 0.47 | 2.09 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:36:ARG:NE | 1:A:41:CYS:SG | 0.47 | 2.87 | 10 | 3 |
| 1:A:36:ARG:HD3 | 1:A:39:PHE:CB | 0.47 | 2.39 | 13 | 1 |
| 1:A:18:GLY:HA2 | 1:A:36:ARG:CD | 0.46 | 2.40 | 11 | 2 |
| 1:A:25:ARG:O | 1:A:29:HIS:HA | 0.46 | 2.11 | 3 | 5 |
| 1:A:8:GLY:O | 1:A:13:PRO:HA | 0.46 | 2.10 | 19 | 1 |
| 1:A:34:ARG:CA | 1:A:41:CYS:HB3 | 0.46 | 2.41 | 13 | 4 |
| 1:A:10:PHE:CD1 | 1:A:11:LYS:HD2 | 0.46 | 2.46 | 8 | 1 |
| 1:A:8:GLY:CA | 1:A:37:ASP:HA | 0.46 | 2.41 | 5 | 2 |
| 1:A:10:PHE:CD2 | 1:A:11:LYS:HD2 | 0.45 | 2.45 | 1 | 1 |
| 1:A:36:ARG:HB3 | 1:A:39:PHE:O | 0.45 | 2.12 | 2 | 1 |
| 1:A:19:ASN:H | 1:A:19:ASN:ND2 | 0.45 | 2.07 | 18 | 4 |
| 1:A:23:HIS:HA | 1:A:27:ASN:ND2 | 0.45 | 2.27 | 15 | 2 |
| 1:A:24:CYS:O | 1:A:29:HIS:N | 0.45 | 2.50 | 12 | 8 |
| 1:A:36:ARG:HG3 | 1:A:41:CYS:HB2 | 0.45 | 1.88 | 13 | 1 |
| 1:A:34:ARG:NE | 1:A:41:CYS:SG | 0.44 | 2.90 | 3 | 1 |
| 1:A:15:ILE:O | 1:A:37:ASP:N | 0.44 | 2.50 | 7 | 1 |
| 1:A:25:ARG:NE | 1:A:33:GLY:HA3 | 0.44 | 2.28 | 20 | 2 |
| 1:A:30:LEU:HD12 | 1:A:43:CYS:HB3 | 0.44 | 1.89 | 7 | 1 |
| 1:A:15:ILE:HD12 | 1:A:19:ASN:HD21 | 0.44 | 1.72 | 10 | 2 |
| 1:A:16:PRO:HA | 1:A:37:ASP:O | 0.44 | 2.13 | 3 | 1 |
| 1:A:19:ASN:HB3 | 1:A:22:LYS:HE3 | 0.44 | 1.90 | 15 | 1 |
| 1:A:19:ASN:HB3 | 1:A:22:LYS:HE2 | 0.44 | 1.90 | 19 | 1 |
| 1:A:19:ASN:HB2 | 1:A:22:LYS:HE3 | 0.43 | 1.88 | 5 | 1 |
| 1:A:25:ARG:HG2 | 1:A:33:GLY:HA3 | 0.43 | 1.89 | 10 | 1 |
| 1:A:21:ASN:HA | 1:A:33:GLY:C | 0.43 | 2.33 | 16 | 1 |
| 1:A:36:ARG:HE | 1:A:39:PHE:HB2 | 0.43 | 1.72 | 15 | 2 |
| 1:A:23:HIS:O | 1:A:27:ASN:ND2 | 0.43 | 2.51 | 14 | 2 |
| 1:A:18:GLY:HA2 | 1:A:36:ARG:HE | 0.43 | 1.74 | 15 | 1 |
| 1:A:20:CYS:SG | 1:A:21:ASN:N | 0.43 | 2.92 | 16 | 1 |
| 1:A:7:SER:OG | 1:A:35:CYS:HA | 0.42 | 2.14 | 7 | 1 |
| 1:A:24:CYS:CB | 1:A:33:GLY:CA | 0.42 | 2.97 | 9 | 2 |
| 1:A:18:GLY:HA3 | 1:A:39:PHE:CD1 | 0.42 | 2.49 | 6 | 1 |
| 1:A:7:SER:HB2 | 1:A:36:ARG:O | 0.42 | 2.15 | 8 | 1 |
| 1:A:6:LEU:CD2 | 1:A:40:ARG:HB3 | 0.42 | 2.45 | 15 | 1 |
| 1:A:10:PHE:O | 1:A:11:LYS:HB2 | 0.42 | 2.15 | 17 | 1 |
| 1:A:19:ASN:N | 1:A:19:ASN:ND2 | 0.42 | 2.66 | 9 | 3 |
| 1:A:25:ARG:N | 1:A:25:ARG:HD3 | 0.42 | 2.29 | 8 | 2 |
| 1:A:30:LEU:HD22 | 1:A:45:ASN:HD22 | 0.42 | 1.75 | 9 | 1 |
| 1:A:30:LEU:CD2 | 1:A:43:CYS:SG | 0.42 | 3.01 | 2 | 1 |
| 1:A:35:CYS:C | 1:A:36:ARG:HG3 | 0.42 | 2.35 | 3 | 1 |
| 1:A:17:ASP:HB3 | 1:A:19:ASN:ND2 | 0.42 | 2.30 | 18 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:5:ASN:ND2 | 1:A:11:LYS:HB3 | 0.42 | 2.30 | 12 | 1 |
| 1:A:15:ILE:HD13 | 1:A:23:HIS:CG | 0.42 | 2.50 | 13 | 2 |
| 1:A:5:ASN:HD21 | 1:A:11:LYS:HB2 | 0.42 | 1.75 | 18 | 1 |
| 1:A:26:ASN:HD22 | 1:A:26:ASN:N | 0.42 | 2.13 | 15 | 1 |
| 1:A:14:CYS:H | 1:A:37:ASP:HB2 | 0.41 | 1.73 | 1 | 1 |
| 1:A:31:LEU:HD13 | 1:A:45:ASN:HA | 0.41 | 1.90 | 11 | 2 |
| 1:A:2:THR:HG1 | 1:A:31:LEU:HD12 | 0.41 | 1.75 | 12 | 1 |
| 1:A:34:ARG:CB | 1:A:41:CYS:CB | 0.41 | 2.94 | 9 | 1 |
| 1:A:6:LEU:O | 1:A:11:LYS:HB3 | 0.41 | 2.15 | 12 | 1 |
| 1:A:6:LEU:HD22 | 1:A:40:ARG:HB2 | 0.41 | 1.92 | 2 | 2 |
| 1:A:30:LEU:N | 1:A:30:LEU:CD1 | 0.41 | 2.83 | 2 | 1 |
| 1:A:18:GLY:HA2 | 1:A:36:ARG:HD3 | 0.41 | 1.91 | 5 | 2 |
| 1:A:19:ASN:CB | 1:A:22:LYS:HE3 | 0.41 | 2.45 | 11 | 1 |
| 1:A:6:LEU:O | 1:A:11:LYS:HB2 | 0.41 | 2.15 | 19 | 1 |
| 1:A:9:THR:HG23 | 1:A:10:PHE:N | 0.41 | 2.31 | 1 | 1 |
| 1:A:18:GLY:N | 1:A:36:ARG:CZ | 0.41 | 2.79 | 7 | 1 |
| 1:A:18:GLY:HA2 | 1:A:39:PHE:CD1 | 0.41 | 2.51 | 9 | 1 |
| 1:A:15:ILE:CD1 | 1:A:19:ASN:HD21 | 0.41 | 2.28 | 14 | 1 |
| 1:A:34:ARG:HG3 | 1:A:42:TRP:O | 0.41 | 2.16 | 8 | 1 |
| 1:A:6:LEU:HD13 | 1:A:10:PHE:CD2 | 0.41 | 2.51 | 18 | 1 |
| 1:A:6:LEU:HG | 1:A:42:TRP:CD1 | 0.41 | 2.50 | 11 | 1 |
| 1:A:34:ARG:H | 1:A:43:CYS:HA | 0.41 | 1.76 | 5 | 1 |
| 1:A:21:ASN:ND2 | 1:A:34:ARG:HG3 | 0.41 | 2.31 | 11 | 1 |
| 1:A:25:ARG:HD3 | 1:A:33:GLY:CA | 0.41 | 2.45 | 11 | 1 |
| 1:A:31:LEU:HB2 | 1:A:44:THR:HB | 0.40 | 1.94 | 10 | 1 |
| 1:A:13:PRO:HB3 | 1:A:37:ASP:OD2 | 0.40 | 2.16 | 9 | 1 |
| 1:A:20:CYS:HB3 | 1:A:36:ARG:HD2 | 0.40 | 1.94 | 9 | 1 |
| 1:A:19:ASN:HB2 | 1:A:22:LYS:HE2 | 0.40 | 1.94 | 10 | 1 |
| 1:A:6:LEU:HD22 | 1:A:40:ARG:HB3 | 0.40 | 1.92 | 14 | 1 |

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-------------|--------------|-------------|------------|-------------|
| 1 | A | 45/47 (96%) | 37±1 (83±3%) | 7±1 (15±3%) | 1±1 (2±2%) | 8 50 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|-----------|----------|-------------|
| All | All | 900/940 (96%) | 748 (83%) | 134 (15%) | 18 (2%) | 8 50 |

All 5 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 | 14 | CYS | 11 |
| 1 | A | 20 | CYS | 3 |
| 1 | A | 9 | THR | 2 |
| 1 | A | 11 | LYS | 1 |
| 1 | A | 38 | ASP | 1 |

6.3.2 Protein sidechains ⓘ

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 | 43/43 (100%) | 37±2 (86±5%) | 6±2 (14±5%) | 5 44 |
| All | All | 860/860 (100%) | 740 (86%) | 120 (14%) | 5 44 |

All 23 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 | 6 | LEU | 20 |
| 1 | A | 19 | ASN | 17 |
| 1 | A | 26 | ASN | 10 |
| 1 | A | 35 | CYS | 10 |
| 1 | A | 41 | CYS | 8 |
| 1 | A | 46 | ARG | 8 |
| 1 | A | 21 | ASN | 7 |
| 1 | A | 2 | THR | 6 |
| 1 | A | 22 | LYS | 4 |
| 1 | A | 14 | CYS | 4 |
| 1 | A | 25 | ARG | 4 |
| 1 | A | 36 | ARG | 3 |
| 1 | A | 27 | ASN | 3 |
| 1 | A | 40 | ARG | 3 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 32 | SER | 2 |
| 1 | A | 24 | CYS | 2 |
| 1 | A | 10 | PHE | 2 |
| 1 | A | 11 | LYS | 2 |
| 1 | A | 17 | ASP | 1 |
| 1 | A | 34 | ARG | 1 |
| 1 | A | 38 | ASP | 1 |
| 1 | A | 15 | ILE | 1 |
| 1 | A | 5 | ASN | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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

| | |
|---|-----|
| Total number of shifts | 489 |
| Number of shifts mapped to atoms | 489 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 1 |

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 47 | -0.03 ± 0.32 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 43 | 0.36 ± 0.45 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 36 | 0.32 ± 0.40 | None needed (< 0.5 ppm) |
| ^{15}N | 37 | 0.90 ± 1.13 | None needed (imprecise) |

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 489 atoms were assigned a chemical shift out of a possible 613. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 209/235 (89%) | 89/96 (93%) | 83/94 (88%) | 37/45 (82%) |
| Sidechain | 260/330 (79%) | 175/207 (85%) | 79/99 (80%) | 6/24 (25%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 20/48 (42%) | 10/24 (42%) | 9/19 (47%) | 1/5 (20%) |
| Overall | 489/613 (80%) | 274/327 (84%) | 171/212 (81%) | 44/74 (59%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 489 atoms were assigned a chemical shift out of a possible 613. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 209/235 (89%) | 89/96 (93%) | 83/94 (88%) | 37/45 (82%) |
| Sidechain | 260/330 (79%) | 175/207 (85%) | 79/99 (80%) | 6/24 (25%) |
| Aromatic | 20/48 (42%) | 10/24 (42%) | 9/19 (47%) | 1/5 (20%) |
| Overall | 489/613 (80%) | 274/327 (84%) | 171/212 (81%) | 44/74 (59%) |

7.1.4 Statistically unusual chemical shifts [i](#)

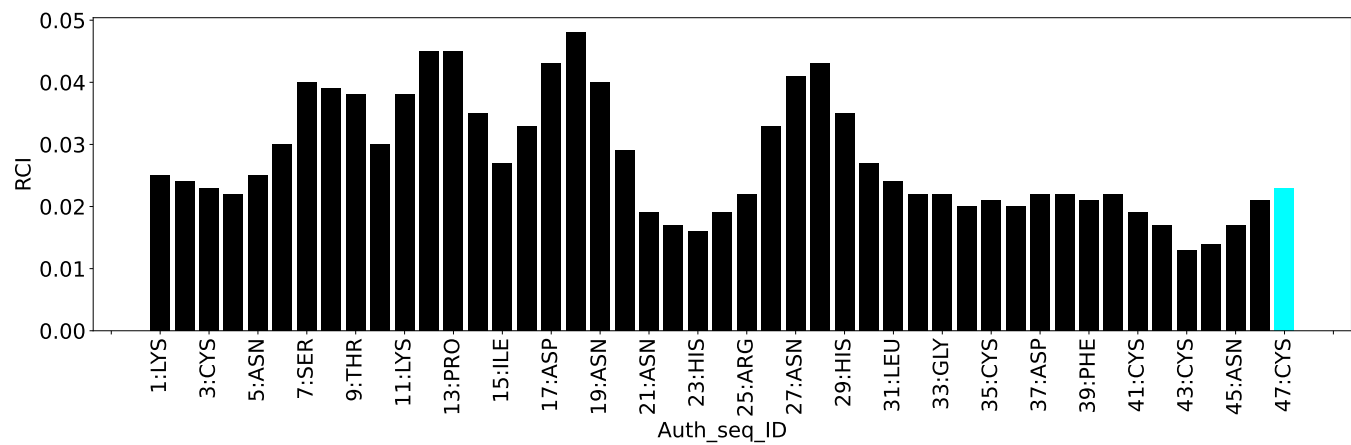
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 40 | ARG | CB | 43.39 | 21.74 – 39.52 | 7.2 |

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 765 |
| Intra-residue ($ i-j =0$) | 359 |
| Sequential ($ i-j =1$) | 141 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 81 |
| Long range ($ i-j \geq 5$) | 162 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 22 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 58 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 17.5 |
| Number of long range restraints per residue ¹ | 3.7 |

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) | 25.2 | 0.2 |
| 0.2-0.5 (Medium) | 42.2 | 0.5 |
| >0.5 (Large) | 48.4 | 3.2 |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 12.9 | 9.91 |
| 10.0-20.0 (Medium) | 1.4 | 17.5 |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

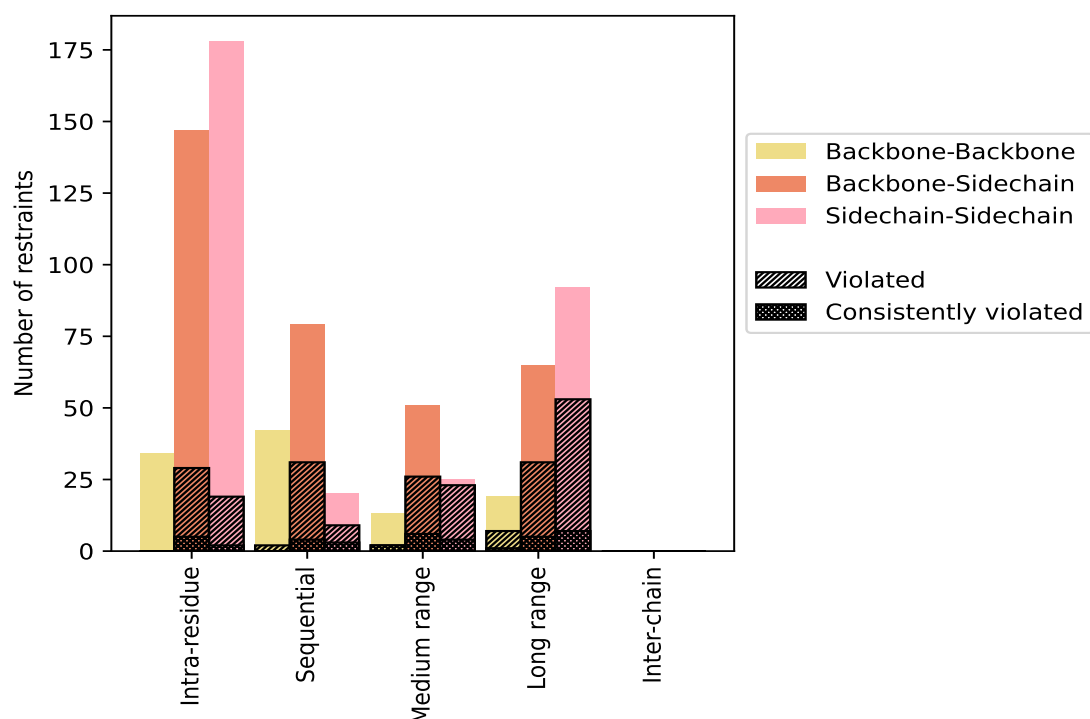
9.1 Summary of distance violations ⓘ

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 359 | 46.9 | 48 | 13.4 | 6.3 | 7 | 1.9 | 0.9 |
| Backbone-Backbone | 34 | 4.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 147 | 19.2 | 29 | 19.7 | 3.8 | 5 | 3.4 | 0.7 |
| Sidechain-Sidechain | 178 | 23.3 | 19 | 10.7 | 2.5 | 2 | 1.1 | 0.3 |
| Sequential ($i-j =1$) | 141 | 18.4 | 42 | 29.8 | 5.5 | 7 | 5.0 | 0.9 |
| Backbone-Backbone | 42 | 5.5 | 2 | 4.8 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 79 | 10.3 | 31 | 39.2 | 4.1 | 4 | 5.1 | 0.5 |
| Sidechain-Sidechain | 20 | 2.6 | 9 | 45.0 | 1.2 | 3 | 15.0 | 0.4 |
| Medium range ($i-j >1$ & $i-j <5$) | 81 | 10.6 | 50 | 61.7 | 6.5 | 12 | 14.8 | 1.6 |
| Backbone-Backbone | 13 | 1.7 | 2 | 15.4 | 0.3 | 2 | 15.4 | 0.3 |
| Backbone-Sidechain | 43 | 5.6 | 25 | 58.1 | 3.3 | 6 | 14.0 | 0.8 |
| Sidechain-Sidechain | 25 | 3.3 | 23 | 92.0 | 3.0 | 4 | 16.0 | 0.5 |
| Long range ($i-j \geq 5$) | 162 | 21.2 | 85 | 52.5 | 11.1 | 12 | 7.4 | 1.6 |
| Backbone-Backbone | 19 | 2.5 | 7 | 36.8 | 0.9 | 1 | 5.3 | 0.1 |
| Backbone-Sidechain | 51 | 6.7 | 25 | 49.0 | 3.3 | 4 | 7.8 | 0.5 |
| Sidechain-Sidechain | 92 | 12.0 | 53 | 57.6 | 6.9 | 7 | 7.6 | 0.9 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 22 | 2.9 | 7 | 31.8 | 0.9 | 1 | 4.5 | 0.1 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 765 | 100.0 | 232 | 30.3 | 30.3 | 39 | 5.1 | 5.1 |
| Backbone-Backbone | 108 | 14.1 | 11 | 10.2 | 1.4 | 3 | 2.8 | 0.4 |
| Backbone-Sidechain | 342 | 44.7 | 117 | 34.2 | 15.3 | 20 | 5.8 | 2.6 |
| Sidechain-Sidechain | 315 | 41.2 | 104 | 33.0 | 13.6 | 16 | 5.1 | 2.1 |

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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 21 | 21 | 26 | 35 | 0 | 103 | 0.58 | 2.8 | 0.54 | 0.39 |
| 2 | 24 | 20 | 26 | 42 | 0 | 112 | 0.66 | 3.2 | 0.59 | 0.46 |
| 3 | 23 | 31 | 29 | 47 | 0 | 130 | 0.56 | 1.8 | 0.44 | 0.43 |
| 4 | 20 | 24 | 31 | 41 | 0 | 116 | 0.53 | 1.84 | 0.4 | 0.42 |
| 5 | 21 | 27 | 31 | 43 | 0 | 122 | 0.6 | 2.68 | 0.53 | 0.44 |
| 6 | 22 | 25 | 29 | 41 | 0 | 117 | 0.59 | 2.33 | 0.48 | 0.42 |
| 7 | 19 | 24 | 30 | 38 | 0 | 111 | 0.53 | 2.1 | 0.43 | 0.44 |
| 8 | 22 | 28 | 27 | 40 | 0 | 117 | 0.54 | 2.19 | 0.44 | 0.39 |
| 9 | 23 | 21 | 29 | 51 | 0 | 124 | 0.55 | 2.28 | 0.46 | 0.42 |
| 10 | 22 | 26 | 33 | 40 | 0 | 121 | 0.59 | 2.19 | 0.48 | 0.42 |

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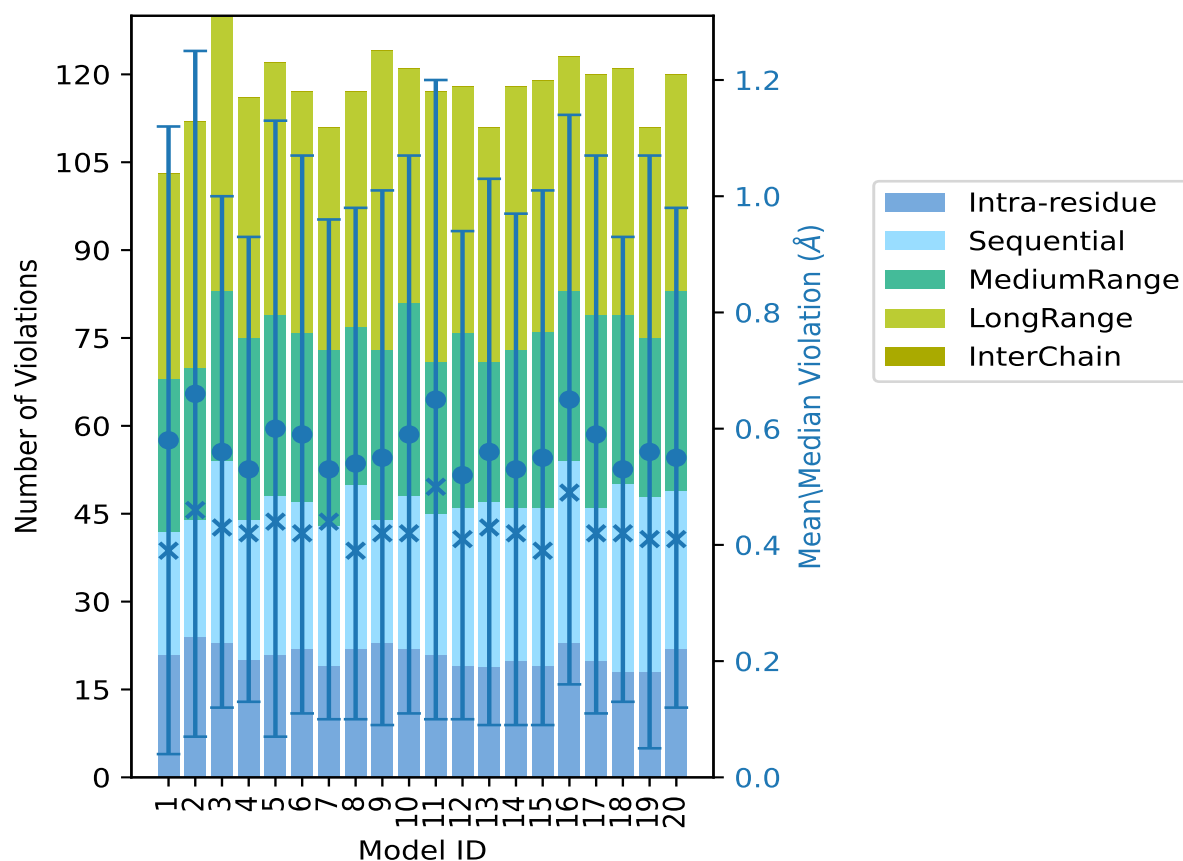
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 21 | 24 | 26 | 46 | 0 | 117 | 0.65 | 2.6 | 0.55 | 0.5 |
| 12 | 19 | 27 | 30 | 42 | 0 | 118 | 0.52 | 2.37 | 0.42 | 0.41 |
| 13 | 19 | 28 | 24 | 40 | 0 | 111 | 0.56 | 2.31 | 0.47 | 0.43 |
| 14 | 20 | 26 | 27 | 45 | 0 | 118 | 0.53 | 1.8 | 0.44 | 0.42 |
| 15 | 19 | 27 | 30 | 43 | 0 | 119 | 0.55 | 2.18 | 0.46 | 0.39 |
| 16 | 23 | 31 | 29 | 40 | 0 | 123 | 0.65 | 1.87 | 0.49 | 0.49 |
| 17 | 20 | 26 | 33 | 41 | 0 | 120 | 0.59 | 2.56 | 0.48 | 0.42 |
| 18 | 18 | 32 | 29 | 42 | 0 | 121 | 0.53 | 1.96 | 0.4 | 0.42 |
| 19 | 18 | 30 | 27 | 36 | 0 | 111 | 0.56 | 2.68 | 0.51 | 0.41 |
| 20 | 22 | 27 | 34 | 37 | 0 | 120 | 0.55 | 2.05 | 0.43 | 0.41 |

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 ⓘ



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

9.3 Distance violation statistics for the ensemble

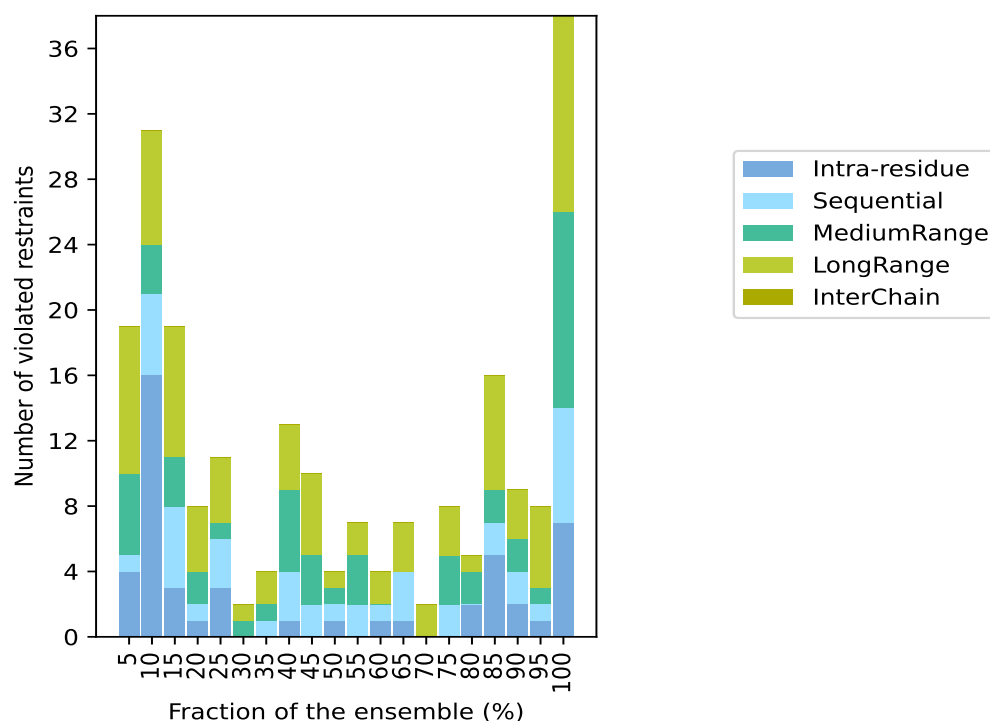
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 518(IR:311, SQ:99, MR:31, LR:77, IC:0) restraints are not 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 | % |
| 4 | 1 | 5 | 9 | 0 | 19 | 1 | 5.0 |
| 16 | 5 | 3 | 7 | 0 | 31 | 2 | 10.0 |
| 3 | 5 | 3 | 8 | 0 | 19 | 3 | 15.0 |
| 1 | 1 | 2 | 4 | 0 | 8 | 4 | 20.0 |
| 3 | 3 | 1 | 4 | 0 | 11 | 5 | 25.0 |
| 0 | 0 | 1 | 1 | 0 | 2 | 6 | 30.0 |
| 0 | 1 | 1 | 2 | 0 | 4 | 7 | 35.0 |
| 1 | 3 | 5 | 4 | 0 | 13 | 8 | 40.0 |
| 0 | 2 | 3 | 5 | 0 | 10 | 9 | 45.0 |
| 1 | 1 | 1 | 1 | 0 | 4 | 10 | 50.0 |
| 0 | 2 | 3 | 2 | 0 | 7 | 11 | 55.0 |
| 1 | 1 | 0 | 2 | 0 | 4 | 12 | 60.0 |
| 1 | 3 | 0 | 3 | 0 | 7 | 13 | 65.0 |
| 0 | 0 | 0 | 2 | 0 | 2 | 14 | 70.0 |
| 0 | 2 | 3 | 3 | 0 | 8 | 15 | 75.0 |
| 2 | 0 | 2 | 1 | 0 | 5 | 16 | 80.0 |
| 5 | 2 | 2 | 7 | 0 | 16 | 17 | 85.0 |
| 2 | 2 | 2 | 3 | 0 | 9 | 18 | 90.0 |
| 1 | 1 | 1 | 5 | 0 | 8 | 19 | 95.0 |
| 7 | 7 | 12 | 12 | 0 | 38 | 20 | 100.0 |

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

⁵Inter-chain restraints, ⁶ Number of models with violations

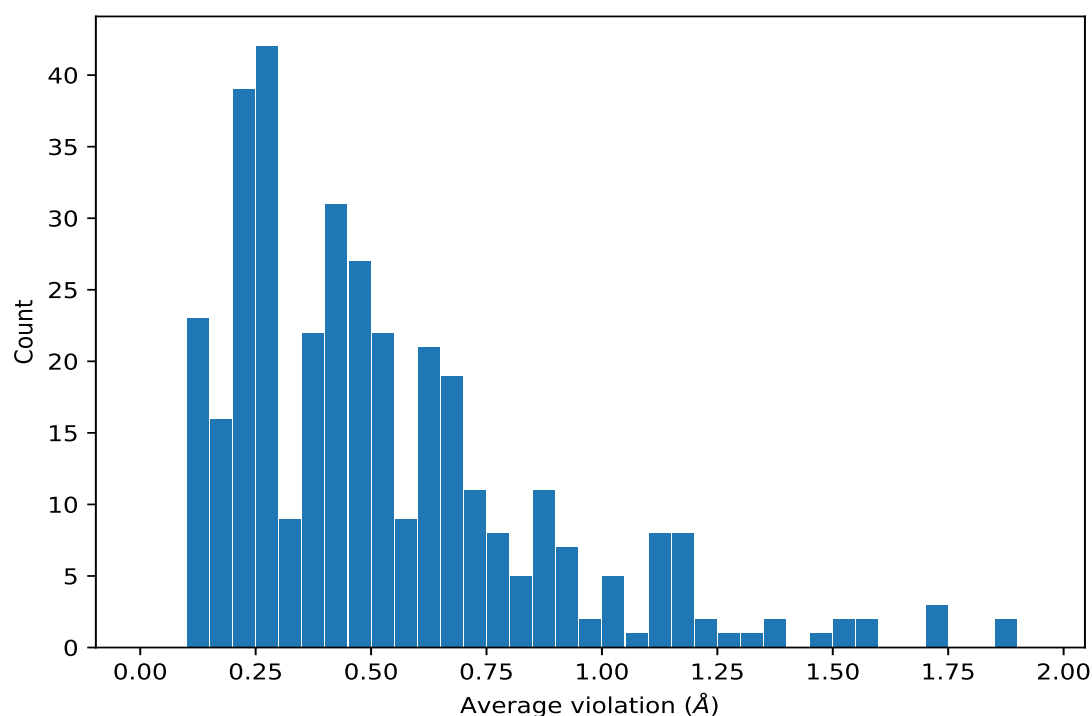
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|---------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 20 | 1.58 | 0.58 | 1.74 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 20 | 1.57 | 0.11 | 1.53 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 20 | 1.18 | 0.36 | 1.35 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 20 | 1.16 | 0.47 | 1.31 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 20 | 1.16 | 0.38 | 1.18 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 20 | 1.15 | 0.58 | 1.4 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB3 | 20 | 1.12 | 0.35 | 1.25 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 20 | 1.12 | 0.35 | 1.25 |
| (2,116) | 1:29:A:HIS:HA | 1:24:A:CYS:HB2 | 20 | 1.12 | 0.35 | 1.25 |
| (2,116) | 1:40:A:ARG:HA | 1:20:A:CYS:HB2 | 20 | 1.12 | 0.35 | 1.25 |
| (1,290) | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3 | 20 | 1.11 | 0.54 | 0.83 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 20 | 1.11 | 0.54 | 0.83 |
| (1,290) | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3 | 20 | 1.11 | 0.54 | 0.83 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 20 | 1.1 | 0.41 | 1.17 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 20 | 1.01 | 0.55 | 1.35 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 20 | 1.0 | 0.16 | 0.97 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG23 | 20 | 1.0 | 0.16 | 0.97 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG21 | 20 | 1.0 | 0.16 | 0.97 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 20 | 0.97 | 0.33 | 1.06 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD11 | 20 | 0.92 | 0.67 | 0.74 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD11 | 20 | 0.92 | 0.67 | 0.74 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD12 | 20 | 0.92 | 0.67 | 0.74 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD13 | 20 | 0.92 | 0.67 | 0.74 |
| (1,286) | 1:44:A:THR:HG21 | 1:30:A:LEU:HD13 | 20 | 0.92 | 0.67 | 0.74 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD13 | 20 | 0.92 | 0.67 | 0.74 |
| (1,238) | 1:6:A:LEU:HD22 | 1:34:A:ARG:HB3 | 20 | 0.86 | 0.39 | 0.62 |
| (1,238) | 1:6:A:LEU:HD21 | 1:34:A:ARG:HB3 | 20 | 0.86 | 0.39 | 0.62 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 20 | 0.86 | 0.39 | 0.62 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 20 | 0.82 | 0.17 | 0.76 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD22 | 20 | 0.81 | 0.6 | 0.5 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 20 | 0.81 | 0.6 | 0.5 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 20 | 0.81 | 0.6 | 0.5 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 20 | 0.8 | 0.47 | 0.64 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 20 | 0.75 | 0.19 | 0.74 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 20 | 0.75 | 0.19 | 0.74 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 20 | 0.75 | 0.16 | 0.74 |
| (2,111) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 20 | 0.75 | 0.16 | 0.74 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD13 | 20 | 0.7 | 0.38 | 0.58 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 20 | 0.7 | 0.38 | 0.58 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD11 | 20 | 0.7 | 0.38 | 0.58 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD11 | 20 | 0.7 | 0.13 | 0.72 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 20 | 0.7 | 0.13 | 0.72 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 20 | 0.7 | 0.13 | 0.72 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD12 | 20 | 0.69 | 0.02 | 0.7 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 20 | 0.69 | 0.02 | 0.7 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 20 | 0.69 | 0.02 | 0.7 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 20 | 0.66 | 0.19 | 0.74 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 20 | 0.66 | 0.19 | 0.74 |
| (1,268) | 1:31:A:LEU:HD23 | 1:44:A:THR:H | 20 | 0.66 | 0.19 | 0.74 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 20 | 0.63 | 0.59 | 0.31 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 20 | 0.62 | 0.17 | 0.63 |
| (2,113) | 1:31:A:LEU:HG | 1:43:A:CYS:HB3 | 20 | 0.62 | 0.17 | 0.63 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 20 | 0.6 | 0.09 | 0.62 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 20 | 0.6 | 0.09 | 0.62 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG23 | 20 | 0.6 | 0.09 | 0.62 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 20 | 0.58 | 0.05 | 0.6 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG21 | 20 | 0.58 | 0.05 | 0.6 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG23 | 20 | 0.58 | 0.05 | 0.6 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 20 | 0.55 | 0.52 | 0.38 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 20 | 0.55 | 0.52 | 0.38 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD23 | 20 | 0.55 | 0.52 | 0.38 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD11 | 20 | 0.54 | 0.23 | 0.48 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD12 | 20 | 0.54 | 0.23 | 0.48 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 20 | 0.54 | 0.23 | 0.48 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 20 | 0.54 | 0.04 | 0.54 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 20 | 0.54 | 0.04 | 0.54 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD23 | 20 | 0.54 | 0.04 | 0.54 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 20 | 0.52 | 0.19 | 0.52 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 20 | 0.49 | 0.07 | 0.48 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 20 | 0.49 | 0.07 | 0.48 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD23 | 20 | 0.49 | 0.07 | 0.48 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 20 | 0.47 | 0.05 | 0.48 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 20 | 0.47 | 0.05 | 0.48 |
| (1,269) | 1:15:A:ILE:HG22 | 1:15:A:ILE:HG13 | 20 | 0.47 | 0.05 | 0.48 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 20 | 0.41 | 0.1 | 0.4 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 20 | 0.35 | 0.11 | 0.36 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 20 | 0.3 | 0.06 | 0.32 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 20 | 0.25 | 0.07 | 0.28 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD2 | 20 | 0.25 | 0.07 | 0.28 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD23 | 20 | 0.24 | 0.02 | 0.24 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD21 | 20 | 0.24 | 0.02 | 0.24 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD23 | 20 | 0.24 | 0.02 | 0.24 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD23 | 20 | 0.24 | 0.02 | 0.24 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD21 | 20 | 0.24 | 0.02 | 0.24 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 20 | 0.24 | 0.02 | 0.24 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD21 | 20 | 0.24 | 0.02 | 0.24 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD22 | 20 | 0.24 | 0.02 | 0.24 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 20 | 0.15 | 0.03 | 0.15 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 19 | 1.34 | 0.45 | 1.43 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 19 | 0.69 | 0.41 | 0.54 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG22 | 19 | 0.69 | 0.41 | 0.54 |
| (2,70) | 1:4:A:GLU:HG3 | 1:30:A:LEU:HD11 | 19 | 0.69 | 0.41 | 0.54 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG23 | 19 | 0.69 | 0.41 | 0.54 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 19 | 0.64 | 0.24 | 0.64 |
| (2,117) | 1:21:A:ASN:H | 1:36:A:ARG:H | 19 | 0.64 | 0.24 | 0.64 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 19 | 0.62 | 0.21 | 0.65 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD22 | 19 | 0.48 | 0.15 | 0.53 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD11 | 19 | 0.48 | 0.15 | 0.53 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD23 | 19 | 0.48 | 0.15 | 0.53 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD21 | 19 | 0.48 | 0.15 | 0.53 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD13 | 19 | 0.48 | 0.15 | 0.53 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 19 | 0.41 | 0.13 | 0.38 |
| (1,350) | 1:2:A:THR:HG22 | 1:46:A:ARG:HB3 | 19 | 0.41 | 0.13 | 0.38 |
| (1,350) | 1:2:A:THR:HG23 | 1:46:A:ARG:HB3 | 19 | 0.41 | 0.13 | 0.38 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 19 | 0.25 | 0.06 | 0.26 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 19 | 0.25 | 0.06 | 0.26 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD2 | 19 | 0.22 | 0.06 | 0.21 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 19 | 0.22 | 0.06 | 0.21 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 18 | 1.87 | 0.4 | 1.9 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 18 | 1.87 | 0.4 | 1.9 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 18 | 0.6 | 0.39 | 0.66 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 18 | 0.52 | 0.31 | 0.52 |
| (2,69) | 1:30:A:LEU:HD23 | 1:28:A:GLU:HB2 | 18 | 0.5 | 0.09 | 0.5 |
| (2,69) | 1:30:A:LEU:HD22 | 1:28:A:GLU:HB2 | 18 | 0.5 | 0.09 | 0.5 |
| (2,69) | 1:30:A:LEU:HD21 | 1:28:A:GLU:HB2 | 18 | 0.5 | 0.09 | 0.5 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD13 | 18 | 0.48 | 0.04 | 0.48 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD12 | 18 | 0.48 | 0.04 | 0.48 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 18 | 0.48 | 0.04 | 0.48 |
| (1,275) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HB2 | 18 | 0.42 | 0.02 | 0.42 |
| (1,275) | 1:30:A:LEU:HD23 | 1:30:A:LEU:HB2 | 18 | 0.42 | 0.02 | 0.42 |
| (1,275) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HB2 | 18 | 0.42 | 0.02 | 0.42 |
| (1,257) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA | 18 | 0.37 | 0.05 | 0.37 |
| (1,257) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA | 18 | 0.37 | 0.05 | 0.37 |
| (1,257) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA | 18 | 0.37 | 0.05 | 0.37 |
| (1,288) | 1:44:A:THR:HG22 | 1:31:A:LEU:HB3 | 18 | 0.35 | 0.06 | 0.36 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 18 | 0.35 | 0.06 | 0.36 |
| (1,288) | 1:44:A:THR:HG21 | 1:31:A:LEU:HB3 | 18 | 0.35 | 0.06 | 0.36 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 18 | 0.33 | 0.22 | 0.28 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 17 | 1.17 | 0.42 | 1.24 |
| (2,114) | 1:9:A:THR:H | 1:14:A:CYS:HB3 | 17 | 1.17 | 0.42 | 1.24 |
| (2,114) | 1:27:A:ASN:HD22 | 1:14:A:CYS:HB3 | 17 | 1.17 | 0.42 | 1.24 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 17 | 0.87 | 0.27 | 0.95 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 17 | 0.79 | 0.78 | 0.14 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 17 | 0.64 | 0.04 | 0.65 |
| (1,282) | 1:30:A:LEU:HD13 | 1:43:A:CYS:HB3 | 17 | 0.64 | 0.78 | 0.38 |
| (1,282) | 1:30:A:LEU:HD12 | 1:43:A:CYS:HB3 | 17 | 0.64 | 0.78 | 0.38 |
| (1,282) | 1:30:A:LEU:HD11 | 1:43:A:CYS:HB3 | 17 | 0.64 | 0.78 | 0.38 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 17 | 0.46 | 0.01 | 0.46 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 17 | 0.43 | 0.13 | 0.37 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 17 | 0.34 | 0.07 | 0.32 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 17 | 0.27 | 0.09 | 0.27 |
| (1,280) | 1:30:A:LEU:HD13 | 1:28:A:GLU:HB3 | 17 | 0.25 | 0.06 | 0.27 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,280) | 1:30:A:LEU:HD11 | 1:28:A:GLU:HB3 | 17 | 0.25 | 0.06 | 0.27 |
| (1,280) | 1:30:A:LEU:HD12 | 1:28:A:GLU:HB3 | 17 | 0.25 | 0.06 | 0.27 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 17 | 0.22 | 0.01 | 0.22 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 17 | 0.19 | 0.04 | 0.19 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 17 | 0.16 | 0.03 | 0.16 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 17 | 0.15 | 0.02 | 0.16 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 17 | 0.15 | 0.01 | 0.15 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 17 | 0.12 | 0.01 | 0.12 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 16 | 1.52 | 0.46 | 1.72 |
| (2,10) | 1:27:A:ASN:HD22 | 1:28:A:GLU:HA | 16 | 1.52 | 0.46 | 1.72 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 16 | 1.17 | 0.44 | 1.21 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 16 | 0.67 | 0.14 | 0.72 |
| (2,32) | 1:30:A:LEU:HD21 | 1:33:A:GLY:H | 16 | 0.39 | 0.11 | 0.38 |
| (2,32) | 1:30:A:LEU:HD23 | 1:33:A:GLY:H | 16 | 0.39 | 0.11 | 0.38 |
| (2,32) | 1:30:A:LEU:HD22 | 1:33:A:GLY:H | 16 | 0.39 | 0.11 | 0.38 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 16 | 0.21 | 0.03 | 0.22 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 16 | 0.16 | 0.03 | 0.16 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 15 | 1.07 | 0.61 | 1.36 |
| (1,489) | 1:30:A:LEU:HD22 | 1:43:A:CYS:HB3 | 15 | 0.88 | 0.11 | 0.89 |
| (1,489) | 1:30:A:LEU:HD23 | 1:43:A:CYS:HB3 | 15 | 0.88 | 0.11 | 0.89 |
| (1,489) | 1:30:A:LEU:HD21 | 1:43:A:CYS:HB3 | 15 | 0.88 | 0.11 | 0.89 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 15 | 0.69 | 0.39 | 0.83 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 15 | 0.43 | 0.26 | 0.35 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 15 | 0.42 | 0.39 | 0.21 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 15 | 0.29 | 0.12 | 0.27 |
| (1,262) | 1:30:A:LEU:HD21 | 1:31:A:LEU:H | 15 | 0.27 | 0.08 | 0.28 |
| (1,262) | 1:30:A:LEU:HD23 | 1:31:A:LEU:H | 15 | 0.27 | 0.08 | 0.28 |
| (1,262) | 1:30:A:LEU:HD22 | 1:31:A:LEU:H | 15 | 0.27 | 0.08 | 0.28 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 15 | 0.26 | 0.07 | 0.28 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG2 | 15 | 0.26 | 0.07 | 0.28 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 15 | 0.23 | 0.07 | 0.26 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 14 | 0.44 | 0.22 | 0.48 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD11 | 14 | 0.42 | 0.22 | 0.44 |
| (2,12) | 1:32:A:SER:H | 1:31:A:LEU:HD13 | 14 | 0.42 | 0.22 | 0.44 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 14 | 0.42 | 0.22 | 0.44 |
| (2,12) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 14 | 0.42 | 0.22 | 0.44 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD12 | 14 | 0.42 | 0.22 | 0.44 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 13 | 1.02 | 1.07 | 0.42 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 13 | 0.48 | 0.41 | 0.15 |
| (2,4) | 1:37:A:ASP:H | 1:15:A:ILE:HG22 | 13 | 0.48 | 0.38 | 0.36 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD12 | 13 | 0.48 | 0.38 | 0.36 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD13 | 13 | 0.48 | 0.38 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,4) | 1:37:A:ASP:H | 1:15:A:ILE:HG21 | 13 | 0.48 | 0.38 | 0.36 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD11 | 13 | 0.48 | 0.38 | 0.36 |
| (2,99) | 1:1:A:LYS:HG2 | 1:1:A:LYS:HA | 13 | 0.47 | 0.03 | 0.47 |
| (2,99) | 1:1:A:LYS:HG3 | 1:1:A:LYS:HA | 13 | 0.47 | 0.03 | 0.47 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 13 | 0.34 | 0.05 | 0.36 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 13 | 0.2 | 0.2 | 0.13 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 13 | 0.14 | 0.02 | 0.14 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 12 | 0.54 | 0.53 | 0.22 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD23 | 12 | 0.41 | 0.18 | 0.39 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD22 | 12 | 0.41 | 0.18 | 0.39 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD21 | 12 | 0.41 | 0.18 | 0.39 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG23 | 12 | 0.26 | 0.05 | 0.28 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG21 | 12 | 0.26 | 0.05 | 0.28 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG22 | 12 | 0.26 | 0.05 | 0.28 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 12 | 0.22 | 0.03 | 0.22 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 11 | 1.28 | 0.47 | 1.47 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE2 | 11 | 0.66 | 0.57 | 0.46 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE3 | 11 | 0.66 | 0.57 | 0.46 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 11 | 0.42 | 0.13 | 0.4 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 11 | 0.42 | 0.48 | 0.14 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 11 | 0.38 | 0.16 | 0.45 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HB2 | 11 | 0.38 | 0.16 | 0.45 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB2 | 11 | 0.29 | 0.17 | 0.24 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB3 | 11 | 0.29 | 0.17 | 0.24 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 11 | 0.23 | 0.13 | 0.19 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 10 | 0.86 | 0.78 | 0.76 |
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 10 | 0.56 | 0.17 | 0.56 |
| (2,91) | 1:7:A:SER:HB3 | 1:34:A:ARG:HB3 | 10 | 0.56 | 0.17 | 0.56 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 10 | 0.27 | 0.13 | 0.2 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 10 | 0.16 | 0.04 | 0.15 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 9 | 1.23 | 0.32 | 1.19 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD11 | 9 | 0.41 | 0.15 | 0.48 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 9 | 0.41 | 0.15 | 0.48 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD12 | 9 | 0.41 | 0.15 | 0.48 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 9 | 0.37 | 0.26 | 0.35 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 9 | 0.36 | 0.18 | 0.41 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 9 | 0.26 | 0.12 | 0.25 |
| (1,191) | 1:10:A:PHE:HD1 | 1:42:A:TRP:HZ2 | 9 | 0.25 | 0.16 | 0.18 |
| (1,191) | 1:10:A:PHE:HD2 | 1:42:A:TRP:HZ2 | 9 | 0.25 | 0.16 | 0.18 |
| (1,300) | 1:2:A:THR:HG21 | 1:46:A:ARG:HG2 | 9 | 0.23 | 0.09 | 0.21 |
| (1,300) | 1:2:A:THR:HG22 | 1:46:A:ARG:HG2 | 9 | 0.23 | 0.09 | 0.21 |
| (1,300) | 1:2:A:THR:HG23 | 1:46:A:ARG:HG2 | 9 | 0.23 | 0.09 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,34) | 1:45:A:ASN:HD21 | 1:30:A:LEU:HB2 | 9 | 0.22 | 0.08 | 0.19 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 9 | 0.22 | 0.08 | 0.19 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 9 | 0.15 | 0.04 | 0.15 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 9 | 0.12 | 0.01 | 0.12 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 8 | 1.47 | 0.24 | 1.54 |
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 8 | 0.94 | 0.2 | 0.94 |
| (1,183) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HB3 | 8 | 0.68 | 0.17 | 0.68 |
| (1,183) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HB3 | 8 | 0.68 | 0.17 | 0.68 |
| (2,98) | 1:32:A:SER:HB2 | 1:34:A:ARG:H | 8 | 0.48 | 0.11 | 0.51 |
| (2,98) | 1:24:A:CYS:HA | 1:26:A:ASN:H | 8 | 0.48 | 0.11 | 0.51 |
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 8 | 0.41 | 0.32 | 0.3 |
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 8 | 0.4 | 0.37 | 0.16 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 8 | 0.37 | 0.13 | 0.38 |
| (1,255) | 1:31:A:LEU:HD11 | 1:4:A:GLU:HB2 | 8 | 0.27 | 0.14 | 0.23 |
| (1,255) | 1:31:A:LEU:HD12 | 1:4:A:GLU:HB2 | 8 | 0.27 | 0.14 | 0.23 |
| (1,255) | 1:31:A:LEU:HD13 | 1:4:A:GLU:HB2 | 8 | 0.27 | 0.14 | 0.23 |
| (1,259) | 1:2:A:THR:HG23 | 1:1:A:LYS:HA | 8 | 0.24 | 0.08 | 0.26 |
| (1,259) | 1:2:A:THR:HG21 | 1:1:A:LYS:HA | 8 | 0.24 | 0.08 | 0.26 |
| (1,259) | 1:2:A:THR:HG22 | 1:1:A:LYS:HA | 8 | 0.24 | 0.08 | 0.26 |
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 8 | 0.2 | 0.05 | 0.18 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 8 | 0.18 | 0.02 | 0.18 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 8 | 0.17 | 0.14 | 0.12 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 8 | 0.14 | 0.03 | 0.14 |
| (1,454) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HA | 7 | 0.98 | 0.7 | 1.45 |
| (1,508) | 1:13:A:PRO:HD2 | 1:12:A:GLY:HA2 | 7 | 0.52 | 0.13 | 0.54 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD21 | 7 | 0.47 | 0.37 | 0.28 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD22 | 7 | 0.47 | 0.37 | 0.28 |
| (1,600) | 1:6:A:LEU:HG | 1:34:A:ARG:HB3 | 7 | 0.34 | 0.09 | 0.38 |
| (2,66) | 1:1:A:LYS:HB2 | 1:4:A:GLU:H | 6 | 0.26 | 0.12 | 0.21 |
| (2,66) | 1:1:A:LYS:HB3 | 1:4:A:GLU:H | 6 | 0.26 | 0.12 | 0.21 |
| (1,529) | 1:33:A:GLY:HA3 | 1:22:A:LYS:HA | 6 | 0.12 | 0.02 | 0.11 |
| (1,250) | 1:31:A:LEU:HD13 | 1:2:A:THR:HG22 | 5 | 0.61 | 0.56 | 0.21 |
| (1,250) | 1:31:A:LEU:HD12 | 1:2:A:THR:HG21 | 5 | 0.61 | 0.56 | 0.21 |
| (1,250) | 1:31:A:LEU:HD11 | 1:2:A:THR:HG21 | 5 | 0.61 | 0.56 | 0.21 |
| (1,250) | 1:31:A:LEU:HD11 | 1:2:A:THR:HG22 | 5 | 0.61 | 0.56 | 0.21 |
| (1,250) | 1:31:A:LEU:HD13 | 1:2:A:THR:HG21 | 5 | 0.61 | 0.56 | 0.21 |
| (2,65) | 1:28:A:GLU:H | 1:28:A:GLU:HG2 | 5 | 0.38 | 0.2 | 0.31 |
| (2,65) | 1:28:A:GLU:H | 1:28:A:GLU:HG3 | 5 | 0.38 | 0.2 | 0.31 |
| (2,65) | 1:22:A:LYS:HB2 | 1:26:A:ASN:HD22 | 5 | 0.38 | 0.2 | 0.31 |
| (1,116) | 1:25:A:ARG:H | 1:26:A:ASN:HB3 | 5 | 0.27 | 0.08 | 0.3 |
| (1,92) | 1:12:A:GLY:H | 1:11:A:LYS:HA | 5 | 0.26 | 0.13 | 0.27 |
| (1,140) | 1:32:A:SER:H | 1:44:A:THR:HG22 | 5 | 0.25 | 0.13 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,140) | 1:32:A:SER:H | 1:44:A:THR:HG23 | 5 | 0.25 | 0.13 | 0.19 |
| (1,140) | 1:32:A:SER:H | 1:44:A:THR:HG21 | 5 | 0.25 | 0.13 | 0.19 |
| (2,67) | 1:13:A:PRO:HG2 | 1:12:A:GLY:H | 5 | 0.25 | 0.07 | 0.23 |
| (2,67) | 1:11:A:LYS:HD3 | 1:12:A:GLY:H | 5 | 0.25 | 0.07 | 0.23 |
| (2,108) | 1:10:A:PHE:H | 1:11:A:LYS:HD3 | 5 | 0.23 | 0.03 | 0.23 |
| (1,598) | 1:46:A:ARG:HG2 | 1:31:A:LEU:HD11 | 5 | 0.22 | 0.06 | 0.2 |
| (1,598) | 1:46:A:ARG:HG2 | 1:31:A:LEU:HD12 | 5 | 0.22 | 0.06 | 0.2 |
| (1,598) | 1:46:A:ARG:HG2 | 1:31:A:LEU:HD13 | 5 | 0.22 | 0.06 | 0.2 |
| (1,364) | 1:34:A:ARG:H | 1:34:A:ARG:HB3 | 5 | 0.15 | 0.03 | 0.13 |
| (1,141) | 1:45:A:ASN:HD21 | 1:30:A:LEU:HB2 | 5 | 0.13 | 0.02 | 0.12 |
| (1,146) | 1:45:A:ASN:HD21 | 1:45:A:ASN:HB3 | 5 | 0.11 | 0.01 | 0.11 |
| (1,495) | 1:10:A:PHE:HD2 | 1:10:A:PHE:HA | 4 | 0.36 | 0.03 | 0.34 |
| (1,495) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HA | 4 | 0.36 | 0.03 | 0.34 |
| (1,249) | 1:31:A:LEU:HD11 | 1:44:A:THR:HG21 | 4 | 0.25 | 0.2 | 0.15 |
| (1,249) | 1:31:A:LEU:HD12 | 1:44:A:THR:HG23 | 4 | 0.25 | 0.2 | 0.15 |
| (1,249) | 1:31:A:LEU:HD11 | 1:44:A:THR:HG23 | 4 | 0.25 | 0.2 | 0.15 |
| (2,20) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HG3 | 4 | 0.22 | 0.09 | 0.2 |
| (2,20) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HB2 | 4 | 0.22 | 0.09 | 0.2 |
| (1,442) | 1:6:A:LEU:HG | 1:34:A:ARG:HD2 | 4 | 0.21 | 0.02 | 0.22 |
| (1,176) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HD3 | 4 | 0.21 | 0.16 | 0.12 |
| (1,176) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HD3 | 4 | 0.21 | 0.16 | 0.12 |
| (1,164) | 1:28:A:GLU:H | 1:27:A:ASN:HB2 | 4 | 0.13 | 0.01 | 0.13 |
| (3,1) | 1:24:A:CYS:H | 1:20:A:CYS:O | 4 | 0.12 | 0.01 | 0.12 |
| (1,412) | 1:36:A:ARG:HG3 | 1:20:A:CYS:HB3 | 4 | 0.12 | 0.02 | 0.12 |
| (1,380) | 1:4:A:GLU:HG3 | 1:32:A:SER:HB2 | 4 | 0.11 | 0.0 | 0.11 |
| (1,587) | 1:24:A:CYS:HA | 1:25:A:ARG:HG2 | 3 | 1.22 | 0.08 | 1.18 |
| (1,82) | 1:6:A:LEU:H | 1:5:A:ASN:HB2 | 3 | 0.88 | 0.07 | 0.92 |
| (1,308) | 1:25:A:ARG:HG2 | 1:25:A:ARG:H | 3 | 0.78 | 0.06 | 0.75 |
| (1,185) | 1:10:A:PHE:HD1 | 1:11:A:LYS:HD3 | 3 | 0.76 | 0.34 | 0.92 |
| (1,185) | 1:10:A:PHE:HD2 | 1:11:A:LYS:HD3 | 3 | 0.76 | 0.34 | 0.92 |
| (2,31) | 1:30:A:LEU:HD13 | 1:33:A:GLY:H | 3 | 0.7 | 0.33 | 0.8 |
| (2,31) | 1:30:A:LEU:HD11 | 1:33:A:GLY:H | 3 | 0.7 | 0.33 | 0.8 |
| (2,31) | 1:30:A:LEU:HD12 | 1:33:A:GLY:H | 3 | 0.7 | 0.33 | 0.8 |
| (1,9) | 1:24:A:CYS:H | 1:43:A:CYS:HB2 | 3 | 0.65 | 0.03 | 0.66 |
| (1,338) | 1:25:A:ARG:HB3 | 1:25:A:ARG:HD2 | 3 | 0.62 | 0.0 | 0.62 |
| (1,178) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB2 | 3 | 0.54 | 0.02 | 0.55 |
| (2,37) | 1:32:A:SER:HA | 1:25:A:ARG:HG2 | 3 | 0.54 | 0.18 | 0.46 |
| (2,37) | 1:32:A:SER:HA | 1:25:A:ARG:HG3 | 3 | 0.54 | 0.18 | 0.46 |
| (2,93) | 1:7:A:SER:HB3 | 1:40:A:ARG:HA | 3 | 0.52 | 0.37 | 0.4 |
| (2,93) | 1:7:A:SER:HB3 | 1:37:A:ASP:HA | 3 | 0.52 | 0.37 | 0.4 |
| (1,272) | 1:15:A:ILE:HD12 | 1:17:A:ASP:HB2 | 3 | 0.37 | 0.2 | 0.34 |
| (1,272) | 1:15:A:ILE:HD13 | 1:17:A:ASP:HB2 | 3 | 0.37 | 0.2 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,429) | 1:46:A:ARG:HD2 | 1:45:A:ASN:HB3 | 3 | 0.25 | 0.08 | 0.31 |
| (1,622) | 1:36:A:ARG:H | 1:15:A:ILE:HG12 | 3 | 0.24 | 0.09 | 0.29 |
| (1,229) | 1:36:A:ARG:HA | 1:15:A:ILE:HD11 | 3 | 0.22 | 0.09 | 0.2 |
| (2,8) | 1:2:A:THR:H | 1:1:A:LYS:HG2 | 3 | 0.18 | 0.04 | 0.21 |
| (1,33) | 1:37:A:ASP:H | 1:39:A:PHE:HB3 | 3 | 0.17 | 0.05 | 0.18 |
| (1,450) | 1:39:A:PHE:HB3 | 1:20:A:CYS:HB3 | 3 | 0.15 | 0.03 | 0.14 |
| (2,97) | 1:8:A:GLY:HA2 | 1:13:A:PRO:HB3 | 3 | 0.15 | 0.05 | 0.13 |
| (3,18) | 1:7:A:SER:N | 1:41:A:CYS:O | 3 | 0.13 | 0.02 | 0.12 |
| (3,20) | 1:32:A:SER:N | 1:44:A:THR:O | 3 | 0.13 | 0.02 | 0.13 |
| (2,3) | 1:33:A:GLY:H | 1:45:A:ASN:HA | 3 | 0.12 | 0.0 | 0.12 |
| (1,284) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HA | 2 | 1.74 | 0.03 | 1.74 |
| (1,284) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HA | 2 | 1.74 | 0.03 | 1.74 |
| (2,22) | 1:21:A:ASN:HD22 | 1:35:A:CYS:H | 2 | 1.74 | 0.1 | 1.74 |
| (1,601) | 1:31:A:LEU:HA | 1:31:A:LEU:HD21 | 2 | 1.38 | 0.03 | 1.38 |
| (1,601) | 1:31:A:LEU:HA | 1:31:A:LEU:HD23 | 2 | 1.38 | 0.03 | 1.38 |
| (1,51) | 1:30:A:LEU:H | 1:30:A:LEU:HD22 | 2 | 0.89 | 0.03 | 0.89 |
| (1,51) | 1:30:A:LEU:H | 1:30:A:LEU:HD23 | 2 | 0.89 | 0.03 | 0.89 |
| (1,253) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB3 | 2 | 0.72 | 0.02 | 0.72 |
| (1,253) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HB3 | 2 | 0.72 | 0.02 | 0.72 |
| (1,351) | 1:30:A:LEU:HD13 | 1:30:A:LEU:HB3 | 2 | 0.66 | 0.02 | 0.66 |
| (1,351) | 1:30:A:LEU:HD12 | 1:30:A:LEU:HB3 | 2 | 0.66 | 0.02 | 0.66 |
| (1,485) | 1:36:A:ARG:HB2 | 1:36:A:ARG:HD2 | 2 | 0.62 | 0.01 | 0.62 |
| (1,620) | 1:22:A:LYS:HB3 | 1:26:A:ASN:HD22 | 2 | 0.56 | 0.45 | 0.56 |
| (1,381) | 1:36:A:ARG:HB3 | 1:40:A:ARG:HA | 2 | 0.54 | 0.38 | 0.54 |
| (1,72) | 1:20:A:CYS:H | 1:21:A:ASN:HB2 | 2 | 0.53 | 0.21 | 0.53 |
| (1,99) | 1:31:A:LEU:H | 1:31:A:LEU:HD22 | 2 | 0.5 | 0.01 | 0.5 |
| (1,99) | 1:31:A:LEU:H | 1:31:A:LEU:HD21 | 2 | 0.5 | 0.01 | 0.5 |
| (2,110) | 1:37:A:ASP:HB2 | 1:38:A:ASP:H | 2 | 0.44 | 0.32 | 0.44 |
| (2,110) | 1:37:A:ASP:HB3 | 1:38:A:ASP:H | 2 | 0.44 | 0.32 | 0.44 |
| (1,472) | 1:36:A:ARG:HB3 | 1:36:A:ARG:HD2 | 2 | 0.41 | 0.0 | 0.41 |
| (2,19) | 1:42:A:TRP:HE3 | 1:11:A:LYS:HD3 | 2 | 0.4 | 0.1 | 0.4 |
| (1,95) | 1:31:A:LEU:H | 1:31:A:LEU:HG | 2 | 0.4 | 0.01 | 0.4 |
| (1,407) | 1:38:A:ASP:HB3 | 1:38:A:ASP:H | 2 | 0.31 | 0.02 | 0.31 |
| (1,156) | 1:45:A:ASN:HD22 | 1:31:A:LEU:HD23 | 2 | 0.3 | 0.04 | 0.3 |
| (1,156) | 1:45:A:ASN:HD22 | 1:31:A:LEU:HD21 | 2 | 0.3 | 0.04 | 0.3 |
| (1,36) | 1:44:A:THR:H | 1:31:A:LEU:HG | 2 | 0.3 | 0.01 | 0.3 |
| (1,53) | 1:30:A:LEU:H | 1:30:A:LEU:HG | 2 | 0.29 | 0.01 | 0.29 |
| (1,492) | 1:20:A:CYS:HB3 | 1:35:A:CYS:HB2 | 2 | 0.28 | 0.13 | 0.28 |
| (1,143) | 1:32:A:SER:H | 1:31:A:LEU:HG | 2 | 0.26 | 0.01 | 0.26 |
| (2,36) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 2 | 0.22 | 0.01 | 0.22 |
| (1,258) | 1:31:A:LEU:HD11 | 1:44:A:THR:HB | 2 | 0.21 | 0.06 | 0.21 |
| (1,258) | 1:31:A:LEU:HD12 | 1:44:A:THR:HB | 2 | 0.21 | 0.06 | 0.21 |

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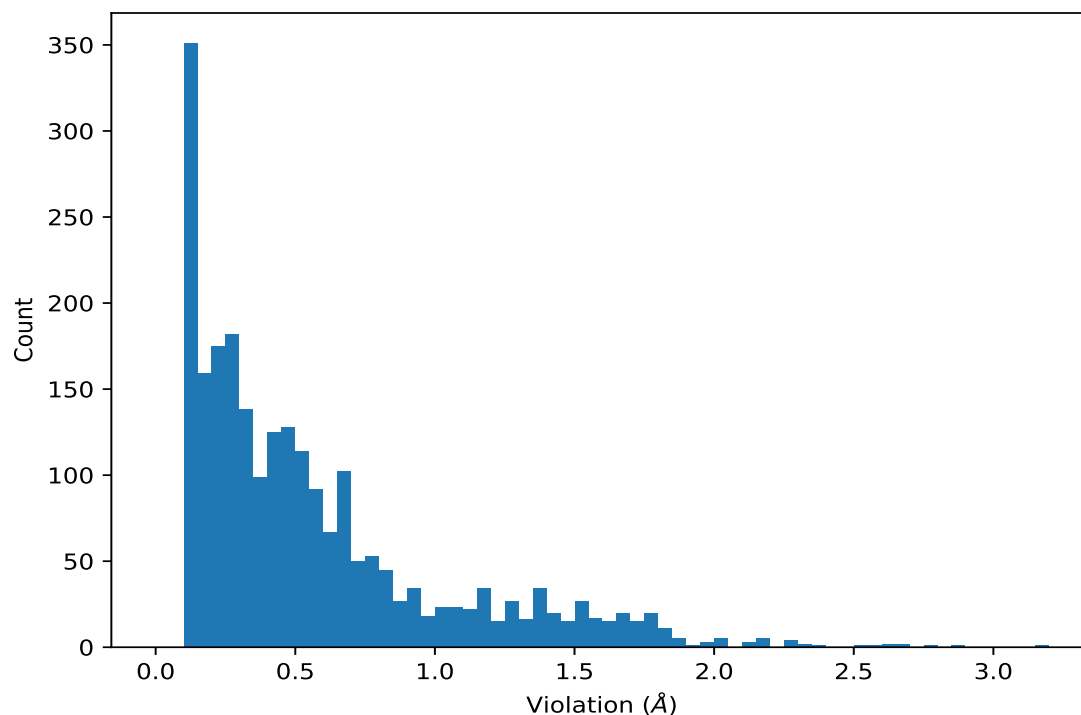
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,298) | 1:11:A:LYS:HG3 | 1:11:A:LYS:HD2 | 2 | 0.16 | 0.02 | 0.16 |
| (2,33) | 1:36:A:ARG:HG2 | 1:20:A:CYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (2,33) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,586) | 1:22:A:LYS:HA | 1:25:A:ARG:HB3 | 2 | 0.12 | 0.01 | 0.12 |
| (2,51) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HD3 | 2 | 0.12 | 0.02 | 0.12 |
| (2,51) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HD2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,432) | 1:46:A:ARG:HB3 | 1:46:A:ARG:HD2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,568) | 1:22:A:LYS:HG2 | 1:22:A:LYS:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,46) | 1:26:A:ASN:H | 1:25:A:ARG:HB3 | 2 | 0.11 | 0.01 | 0.11 |
| (1,378) | 1:4:A:GLU:HG3 | 1:5:A:ASN:HB3 | 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

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) |
|---------|-----------------|-----------------|----------|---------------|
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD11 | 2 | 3.2 |
| (1,282) | 1:30:A:LEU:HD13 | 1:43:A:CYS:HB3 | 2 | 2.86 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 1 | 2.8 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 19 | 2.68 |
| (1,282) | 1:30:A:LEU:HD12 | 1:43:A:CYS:HB3 | 5 | 2.68 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 1 | 2.6 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 11 | 2.6 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 17 | 2.56 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD13 | 5 | 2.54 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 12 | 2.37 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 6 | 2.33 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 13 | 2.31 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 2 | 2.29 |
| (2,114) | 1:9:A:THR:H | 1:14:A:CYS:HB3 | 9 | 2.28 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 1 | 2.27 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 13 | 2.27 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 8 | 2.19 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 10 | 2.19 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 10 | 2.18 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 15 | 2.18 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 11 | 2.15 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 11 | 2.14 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 19 | 2.13 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 7 | 2.1 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 20 | 2.05 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 9 | 2.05 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 11 | 2.04 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 7 | 2.0 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 5 | 2.0 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 11 | 1.99 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 15 | 1.97 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 18 | 1.96 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 20 | 1.91 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 1 | 1.9 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 15 | 1.9 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 17 | 1.89 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE3 | 16 | 1.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 5 | 1.87 |
| (2,22) | 1:21:A:ASN:HD22 | 1:35:A:CYS:H | 16 | 1.84 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 4 | 1.84 |
| (2,10) | 1:27:A:ASN:HD22 | 1:28:A:GLU:HA | 16 | 1.83 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 18 | 1.83 |
| (1,190) | 1:10:A:PHE:HD1 | 1:5:A:ASN:HD22 | 8 | 1.83 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 6 | 1.82 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 13 | 1.82 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 16 | 1.81 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 10 | 1.81 |
| (2,10) | 1:27:A:ASN:HD22 | 1:28:A:GLU:HA | 3 | 1.8 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 14 | 1.8 |
| (2,10) | 1:27:A:ASN:HD22 | 1:28:A:GLU:HA | 20 | 1.79 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 6 | 1.79 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 16 | 1.79 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 6 | 1.79 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 19 | 1.79 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 7 | 1.78 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 11 | 1.78 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 11 | 1.78 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 8 | 1.77 |
| (1,454) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HA | 5 | 1.77 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 13 | 1.77 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 2 | 1.77 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 16 | 1.77 |
| (1,284) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HA | 2 | 1.77 |
| (2,10) | 1:27:A:ASN:HD22 | 1:28:A:GLU:HA | 13 | 1.76 |
| (2,10) | 1:27:A:ASN:HD22 | 1:28:A:GLU:HA | 18 | 1.76 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 17 | 1.76 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 15 | 1.75 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 19 | 1.75 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 10 | 1.75 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 16 | 1.74 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 14 | 1.74 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 5 | 1.73 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 6 | 1.73 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 15 | 1.73 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 11 | 1.73 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 17 | 1.73 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 3 | 1.73 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 13 | 1.73 |
| (2,10) | 1:27:A:ASN:HD22 | 1:28:A:GLU:HA | 10 | 1.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 3 | 1.72 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 16 | 1.72 |
| (1,284) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HA | 5 | 1.72 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 3 | 1.72 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 8 | 1.71 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 12 | 1.7 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 11 | 1.7 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 7 | 1.7 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 13 | 1.7 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 9 | 1.7 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 2 | 1.7 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 15 | 1.69 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 5 | 1.69 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 5 | 1.69 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 2 | 1.69 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 6 | 1.68 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 14 | 1.68 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 4 | 1.67 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 19 | 1.67 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 3 | 1.66 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 19 | 1.66 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 17 | 1.66 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 3 | 1.66 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 11 | 1.66 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 9 | 1.66 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 1 | 1.65 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD11 | 10 | 1.65 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 19 | 1.65 |
| (2,22) | 1:21:A:ASN:HD22 | 1:35:A:CYS:H | 1 | 1.64 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 2 | 1.64 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 15 | 1.64 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 20 | 1.64 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 19 | 1.64 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 17 | 1.63 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 11 | 1.62 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 17 | 1.62 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 6 | 1.61 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 17 | 1.61 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 10 | 1.61 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 16 | 1.6 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 10 | 1.59 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 12 | 1.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 1 | 1.59 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 1 | 1.59 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 4 | 1.59 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 15 | 1.59 |
| (2,116) | 1:40:A:ARG:HA | 1:20:A:CYS:HB2 | 9 | 1.58 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 13 | 1.58 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 14 | 1.57 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 16 | 1.57 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 14 | 1.56 |
| (1,454) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HA | 9 | 1.56 |
| (1,454) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HA | 12 | 1.56 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 2 | 1.56 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 16 | 1.56 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 8 | 1.56 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 17 | 1.55 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 9 | 1.54 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 19 | 1.54 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 18 | 1.54 |
| (2,70) | 1:4:A:GLU:HG3 | 1:30:A:LEU:HD11 | 9 | 1.53 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 20 | 1.53 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 4 | 1.53 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 12 | 1.53 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 20 | 1.53 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 14 | 1.53 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 16 | 1.53 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 1 | 1.52 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 8 | 1.52 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 14 | 1.52 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 14 | 1.52 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 20 | 1.52 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 8 | 1.52 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 10 | 1.52 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 7 | 1.52 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 7 | 1.51 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 18 | 1.51 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 8 | 1.51 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 10 | 1.51 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 16 | 1.51 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 11 | 1.5 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 19 | 1.5 |
| (1,290) | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3 | 19 | 1.5 |
| (1,250) | 1:31:A:LEU:HD12 | 1:2:A:THR:HG21 | 11 | 1.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 9 | 1.49 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 3 | 1.49 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 2 | 1.48 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 6 | 1.48 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 6 | 1.48 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 5 | 1.47 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 20 | 1.47 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 2 | 1.47 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 8 | 1.47 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 17 | 1.47 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 2 | 1.46 |
| (1,238) | 1:6:A:LEU:HD21 | 1:34:A:ARG:HB3 | 6 | 1.46 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 7 | 1.46 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 4 | 1.46 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 12 | 1.46 |
| (1,454) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HA | 17 | 1.45 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 14 | 1.44 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 3 | 1.44 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 5 | 1.44 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 9 | 1.44 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE2 | 19 | 1.43 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 13 | 1.43 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 16 | 1.43 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 2 | 1.43 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 8 | 1.43 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 13 | 1.43 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 10 | 1.43 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 4 | 1.42 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 9 | 1.42 |
| (1,601) | 1:31:A:LEU:HA | 1:31:A:LEU:HD21 | 10 | 1.42 |
| (2,114) | 1:9:A:THR:H | 1:14:A:CYS:HB3 | 5 | 1.41 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 18 | 1.41 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 3 | 1.41 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 12 | 1.41 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 16 | 1.41 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 17 | 1.4 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 3 | 1.4 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 2 | 1.4 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 12 | 1.4 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 15 | 1.4 |
| (1,238) | 1:6:A:LEU:HD21 | 1:34:A:ARG:HB3 | 2 | 1.4 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 19 | 1.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 1 | 1.39 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 15 | 1.39 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 15 | 1.38 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 16 | 1.38 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 2 | 1.38 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 10 | 1.38 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 1 | 1.38 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 11 | 1.38 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 18 | 1.38 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 11 | 1.38 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 10 | 1.38 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 5 | 1.37 |
| (1,527) | 1:18:A:GLY:HA3 | 1:20:A:CYS:HB2 | 3 | 1.37 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 6 | 1.36 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 4 | 1.36 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 17 | 1.36 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 20 | 1.36 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 4 | 1.36 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG22 | 2 | 1.35 |
| (2,4) | 1:37:A:ASP:H | 1:15:A:ILE:HG22 | 2 | 1.35 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 11 | 1.35 |
| (1,601) | 1:31:A:LEU:HA | 1:31:A:LEU:HD23 | 11 | 1.35 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 14 | 1.35 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 19 | 1.35 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 6 | 1.35 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 18 | 1.35 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 3 | 1.35 |
| (2,4) | 1:37:A:ASP:H | 1:15:A:ILE:HG21 | 5 | 1.34 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 9 | 1.34 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 16 | 1.34 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 6 | 1.34 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 10 | 1.33 |
| (1,587) | 1:24:A:CYS:HA | 1:25:A:ARG:HG2 | 16 | 1.33 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 20 | 1.32 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 16 | 1.31 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 17 | 1.31 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 11 | 1.31 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 1 | 1.31 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 3 | 1.31 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 9 | 1.31 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 17 | 1.3 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 12 | 1.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 18 | 1.3 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB3 | 18 | 1.29 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 18 | 1.29 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 6 | 1.29 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 2 | 1.29 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 20 | 1.29 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB3 | 10 | 1.28 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 14 | 1.28 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 14 | 1.28 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 9 | 1.28 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 15 | 1.28 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 5 | 1.28 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 13 | 1.27 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 20 | 1.27 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 2 | 1.27 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 20 | 1.27 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 2 | 1.26 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 11 | 1.26 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 12 | 1.26 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG22 | 11 | 1.26 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 14 | 1.26 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 16 | 1.26 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 7 | 1.25 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 15 | 1.25 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 17 | 1.25 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 7 | 1.25 |
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 17 | 1.25 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 16 | 1.25 |
| (2,116) | 1:29:A:HIS:HA | 1:24:A:CYS:HB2 | 8 | 1.24 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 10 | 1.24 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 3 | 1.24 |
| (1,238) | 1:6:A:LEU:HD21 | 1:34:A:ARG:HB3 | 14 | 1.24 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 3 | 1.23 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 4 | 1.23 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 20 | 1.23 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 1 | 1.23 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB3 | 1 | 1.22 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 6 | 1.22 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 4 | 1.22 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 7 | 1.22 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 8 | 1.21 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 8 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 17 | 1.21 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 4 | 1.2 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 11 | 1.2 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 2 | 1.2 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 11 | 1.2 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 6 | 1.2 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 15 | 1.2 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 7 | 1.2 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 12 | 1.2 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 16 | 1.19 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 13 | 1.19 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 6 | 1.19 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 5 | 1.19 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 8 | 1.19 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 12 | 1.19 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 4 | 1.19 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD11 | 2 | 1.19 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 19 | 1.18 |
| (1,587) | 1:24:A:CYS:HA | 1:25:A:ARG:HG2 | 20 | 1.18 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 4 | 1.18 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 14 | 1.18 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG23 | 14 | 1.18 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 20 | 1.18 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 13 | 1.18 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 3 | 1.17 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 5 | 1.17 |
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 12 | 1.17 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG23 | 6 | 1.17 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 8 | 1.17 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 18 | 1.17 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 7 | 1.16 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 20 | 1.16 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG23 | 3 | 1.16 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG23 | 19 | 1.16 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 5 | 1.16 |
| (2,114) | 1:9:A:THR:H | 1:14:A:CYS:HB3 | 6 | 1.15 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE2 | 2 | 1.15 |
| (1,587) | 1:24:A:CYS:HA | 1:25:A:ARG:HG2 | 8 | 1.15 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 15 | 1.15 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 12 | 1.15 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 8 | 1.15 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 3 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 6 | 1.14 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 1 | 1.14 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 10 | 1.14 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 16 | 1.14 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 9 | 1.14 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 5 | 1.14 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 10 | 1.13 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 1 | 1.12 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 4 | 1.12 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 6 | 1.12 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 5 | 1.11 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 3 | 1.11 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG23 | 15 | 1.1 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 1 | 1.1 |
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 3 | 1.1 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 9 | 1.09 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 14 | 1.09 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 18 | 1.09 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG23 | 10 | 1.09 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 7 | 1.09 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG21 | 9 | 1.08 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 2 | 1.08 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 10 | 1.08 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 16 | 1.07 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 8 | 1.07 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 4 | 1.07 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 10 | 1.07 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 17 | 1.07 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 4 | 1.07 |
| (1,185) | 1:10:A:PHE:HD2 | 1:11:A:LYS:HD3 | 3 | 1.07 |
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 16 | 1.06 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 7 | 1.06 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD21 | 11 | 1.06 |
| (2,31) | 1:30:A:LEU:HD13 | 1:33:A:GLY:H | 2 | 1.05 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 18 | 1.05 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 12 | 1.05 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 9 | 1.05 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 5 | 1.05 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 3 | 1.04 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 9 | 1.04 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 12 | 1.04 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 20 | 1.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 15 | 1.04 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 18 | 1.03 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 8 | 1.03 |
| (1,250) | 1:31:A:LEU:HD13 | 1:2:A:THR:HG22 | 10 | 1.03 |
| (2,93) | 1:7:A:SER:HB3 | 1:37:A:ASP:HA | 19 | 1.02 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 7 | 1.02 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 18 | 1.02 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 3 | 1.02 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 15 | 1.02 |
| (1,620) | 1:22:A:LYS:HB3 | 1:26:A:ASN:HD22 | 17 | 1.01 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 7 | 1.01 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 19 | 1.01 |
| (1,446) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG3 | 5 | 1.01 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD22 | 10 | 1.01 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 2 | 1.01 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 6 | 1.0 |
| (1,489) | 1:30:A:LEU:HD22 | 1:43:A:CYS:HB3 | 16 | 1.0 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 5 | 1.0 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 6 | 1.0 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 15 | 0.99 |
| (1,489) | 1:30:A:LEU:HD23 | 1:43:A:CYS:HB3 | 9 | 0.99 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 3 | 0.99 |
| (2,116) | 1:29:A:HIS:HA | 1:24:A:CYS:HB2 | 16 | 0.98 |
| (1,489) | 1:30:A:LEU:HD22 | 1:43:A:CYS:HB3 | 3 | 0.98 |
| (1,489) | 1:30:A:LEU:HD21 | 1:43:A:CYS:HB3 | 14 | 0.98 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 5 | 0.98 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 11 | 0.98 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 20 | 0.98 |
| (2,114) | 1:27:A:ASN:HD22 | 1:14:A:CYS:HB3 | 14 | 0.97 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 18 | 0.97 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 4 | 0.97 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 11 | 0.97 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 11 | 0.97 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 17 | 0.96 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 2 | 0.96 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG21 | 5 | 0.96 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 6 | 0.96 |
| (2,111) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 19 | 0.95 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 16 | 0.95 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 16 | 0.95 |
| (1,489) | 1:30:A:LEU:HD21 | 1:43:A:CYS:HB3 | 6 | 0.95 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 1 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 11 | 0.95 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 3 | 0.95 |
| (1,183) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HB3 | 6 | 0.95 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 12 | 0.94 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 18 | 0.94 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 4 | 0.94 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 13 | 0.94 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 14 | 0.94 |
| (1,82) | 1:6:A:LEU:H | 1:5:A:ASN:HB2 | 16 | 0.94 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 20 | 0.93 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 17 | 0.93 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 12 | 0.93 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD11 | 3 | 0.93 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 10 | 0.93 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 11 | 0.93 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 9 | 0.92 |
| (1,489) | 1:30:A:LEU:HD22 | 1:43:A:CYS:HB3 | 8 | 0.92 |
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 5 | 0.92 |
| (1,381) | 1:36:A:ARG:HB3 | 1:40:A:ARG:HA | 3 | 0.92 |
| (1,185) | 1:10:A:PHE:HD1 | 1:11:A:LYS:HD3 | 16 | 0.92 |
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 2 | 0.92 |
| (1,82) | 1:6:A:LEU:H | 1:5:A:ASN:HB2 | 18 | 0.92 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 9 | 0.92 |
| (1,51) | 1:30:A:LEU:H | 1:30:A:LEU:HD23 | 5 | 0.92 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 5 | 0.91 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 7 | 0.91 |
| (1,489) | 1:30:A:LEU:HD23 | 1:43:A:CYS:HB3 | 15 | 0.91 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 1 | 0.91 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 19 | 0.9 |
| (2,114) | 1:9:A:THR:H | 1:14:A:CYS:HB3 | 11 | 0.89 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 12 | 0.89 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 20 | 0.89 |
| (1,489) | 1:30:A:LEU:HD21 | 1:43:A:CYS:HB3 | 18 | 0.89 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 4 | 0.89 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 7 | 0.89 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 15 | 0.88 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD11 | 16 | 0.88 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 19 | 0.88 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 12 | 0.88 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 16 | 0.88 |
| (1,290) | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3 | 5 | 0.88 |
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 14 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 11 | 0.87 |
| (1,489) | 1:30:A:LEU:HD23 | 1:43:A:CYS:HB3 | 20 | 0.87 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 6 | 0.87 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 15 | 0.87 |
| (2,117) | 1:21:A:ASN:H | 1:36:A:ARG:H | 11 | 0.86 |
| (2,114) | 1:21:A:ASN:HD21 | 1:36:A:ARG:HD3 | 20 | 0.86 |
| (2,111) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 11 | 0.86 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 11 | 0.86 |
| (1,489) | 1:30:A:LEU:HD23 | 1:43:A:CYS:HB3 | 4 | 0.86 |
| (1,489) | 1:30:A:LEU:HD21 | 1:43:A:CYS:HB3 | 10 | 0.86 |
| (1,489) | 1:30:A:LEU:HD21 | 1:43:A:CYS:HB3 | 13 | 0.86 |
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 9 | 0.86 |
| (1,308) | 1:25:A:ARG:HG2 | 1:25:A:ARG:H | 16 | 0.86 |
| (1,51) | 1:30:A:LEU:H | 1:30:A:LEU:HD22 | 2 | 0.86 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 1 | 0.85 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 13 | 0.85 |
| (1,489) | 1:30:A:LEU:HD22 | 1:43:A:CYS:HB3 | 17 | 0.85 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 6 | 0.85 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 16 | 0.85 |
| (1,290) | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3 | 17 | 0.85 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 13 | 0.85 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 14 | 0.85 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 7 | 0.84 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 3 | 0.84 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 9 | 0.84 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 2 | 0.84 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG23 | 2 | 0.84 |
| (1,183) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HB3 | 10 | 0.84 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 11 | 0.84 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 3 | 0.83 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 4 | 0.83 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 9 | 0.83 |
| (1,290) | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3 | 1 | 0.83 |
| (1,290) | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3 | 9 | 0.83 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD13 | 17 | 0.83 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 17 | 0.83 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 6 | 0.83 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 13 | 0.83 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE2 | 4 | 0.82 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 4 | 0.82 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 5 | 0.82 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG21 | 8 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 14 | 0.82 |
| (2,114) | 1:9:A:THR:H | 1:14:A:CYS:HB3 | 13 | 0.81 |
| (2,111) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 2 | 0.81 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 14 | 0.81 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG22 | 4 | 0.81 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG23 | 7 | 0.81 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 15 | 0.81 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD11 | 15 | 0.81 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 19 | 0.8 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 10 | 0.8 |
| (2,31) | 1:30:A:LEU:HD12 | 1:33:A:GLY:H | 5 | 0.8 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD11 | 1 | 0.8 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 17 | 0.8 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 17 | 0.8 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG21 | 13 | 0.8 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 12 | 0.8 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 2 | 0.8 |
| (2,37) | 1:32:A:SER:HA | 1:25:A:ARG:HG2 | 12 | 0.79 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 8 | 0.79 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 14 | 0.79 |
| (1,334) | 1:4:A:GLU:HB2 | 1:2:A:THR:HG21 | 18 | 0.79 |
| (1,290) | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3 | 14 | 0.79 |
| (1,286) | 1:44:A:THR:HG21 | 1:30:A:LEU:HD13 | 9 | 0.79 |
| (1,286) | 1:44:A:THR:HG21 | 1:30:A:LEU:HD13 | 14 | 0.79 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD12 | 18 | 0.79 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 2 | 0.79 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 3 | 0.79 |
| (1,82) | 1:6:A:LEU:H | 1:5:A:ASN:HB2 | 12 | 0.79 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 16 | 0.78 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 6 | 0.78 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 20 | 0.78 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 13 | 0.78 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 13 | 0.78 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 7 | 0.78 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 14 | 0.77 |
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 15 | 0.77 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 10 | 0.77 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 15 | 0.77 |
| (1,268) | 1:31:A:LEU:HD23 | 1:44:A:THR:H | 19 | 0.77 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 9 | 0.77 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 17 | 0.76 |
| (2,110) | 1:37:A:ASP:HB2 | 1:38:A:ASP:H | 19 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 9 | 0.76 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 2 | 0.76 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 13 | 0.76 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 20 | 0.76 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 7 | 0.76 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 18 | 0.76 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 7 | 0.76 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 13 | 0.76 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD13 | 6 | 0.76 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 9 | 0.76 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 12 | 0.76 |
| (1,268) | 1:31:A:LEU:HD23 | 1:44:A:THR:H | 15 | 0.76 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 18 | 0.76 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 15 | 0.75 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 20 | 0.75 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 10 | 0.75 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 17 | 0.75 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 9 | 0.75 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 13 | 0.75 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 20 | 0.75 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 11 | 0.75 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 4 | 0.75 |
| (1,308) | 1:25:A:ARG:HG2 | 1:25:A:ARG:H | 20 | 0.75 |
| (1,290) | 1:9:A:THR:HG21 | 1:11:A:LYS:HD3 | 2 | 0.75 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 7 | 0.75 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD12 | 4 | 0.75 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 9 | 0.75 |
| (1,183) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HB3 | 18 | 0.75 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 17 | 0.74 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 8 | 0.74 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 17 | 0.74 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 12 | 0.74 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 1 | 0.74 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 8 | 0.74 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 19 | 0.74 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 3 | 0.74 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 11 | 0.74 |
| (1,286) | 1:44:A:THR:HG21 | 1:30:A:LEU:HD13 | 12 | 0.74 |
| (1,253) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HB3 | 11 | 0.74 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD23 | 1 | 0.74 |
| (1,72) | 1:20:A:CYS:H | 1:21:A:ASN:HB2 | 16 | 0.74 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 10 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 16 | 0.73 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 5 | 0.73 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 6 | 0.73 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 13 | 0.73 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 18 | 0.73 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 10 | 0.73 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 1 | 0.73 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 19 | 0.73 |
| (1,308) | 1:25:A:ARG:HG2 | 1:25:A:ARG:H | 8 | 0.73 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 6 | 0.73 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 16 | 0.73 |
| (2,69) | 1:30:A:LEU:HD23 | 1:28:A:GLU:HB2 | 17 | 0.72 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB2 | 10 | 0.72 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 9 | 0.72 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 13 | 0.72 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 9 | 0.72 |
| (1,489) | 1:30:A:LEU:HD23 | 1:43:A:CYS:HB3 | 11 | 0.72 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 2 | 0.72 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 8 | 0.72 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 11 | 0.72 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 18 | 0.72 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 3 | 0.72 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 6 | 0.72 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 10 | 0.72 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 14 | 0.72 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD11 | 13 | 0.72 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG23 | 20 | 0.71 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD11 | 15 | 0.71 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 16 | 0.71 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 2 | 0.71 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 9 | 0.71 |
| (1,290) | 1:9:A:THR:HG23 | 1:11:A:LYS:HD3 | 10 | 0.71 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD13 | 19 | 0.71 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 4 | 0.71 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 5 | 0.71 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 4 | 0.71 |
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 16 | 0.7 |
| (2,70) | 1:4:A:GLU:HG3 | 1:30:A:LEU:HD11 | 7 | 0.7 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 18 | 0.7 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 8 | 0.7 |
| (1,508) | 1:13:A:PRO:HD2 | 1:12:A:GLY:HA2 | 15 | 0.7 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 4 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 5 | 0.7 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 9 | 0.7 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD12 | 15 | 0.7 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 20 | 0.7 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 11 | 0.7 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 5 | 0.7 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 17 | 0.7 |
| (1,290) | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3 | 13 | 0.7 |
| (1,268) | 1:31:A:LEU:HD23 | 1:44:A:THR:H | 7 | 0.7 |
| (1,253) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HB3 | 10 | 0.7 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 17 | 0.7 |
| (1,183) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HB3 | 12 | 0.7 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 11 | 0.7 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 17 | 0.7 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 16 | 0.7 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG23 | 12 | 0.7 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 2 | 0.69 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 13 | 0.69 |
| (2,114) | 1:9:A:THR:H | 1:14:A:CYS:HB3 | 3 | 0.69 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 2 | 0.69 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 4 | 0.69 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 5 | 0.69 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 6 | 0.69 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 12 | 0.69 |
| (2,12) | 1:32:A:SER:H | 1:31:A:LEU:HD13 | 2 | 0.69 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 12 | 0.69 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 17 | 0.69 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 19 | 0.69 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 3 | 0.69 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD12 | 7 | 0.69 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 13 | 0.69 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 13 | 0.69 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD13 | 11 | 0.69 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 5 | 0.69 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 6 | 0.69 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 18 | 0.69 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 13 | 0.68 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 6 | 0.68 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 14 | 0.68 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 3 | 0.68 |
| (1,351) | 1:30:A:LEU:HD13 | 1:30:A:LEU:HB3 | 2 | 0.68 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 10 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD12 | 16 | 0.68 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 17 | 0.68 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 20 | 0.68 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 1 | 0.68 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 16 | 0.68 |
| (1,9) | 1:24:A:CYS:H | 1:43:A:CYS:HB2 | 7 | 0.68 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 14 | 0.67 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD12 | 9 | 0.67 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 20 | 0.67 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD12 | 1 | 0.67 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 12 | 0.67 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD12 | 16 | 0.67 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 3 | 0.67 |
| (1,369) | 1:1:A:LYS:HD3 | 1:4:A:GLU:HB3 | 13 | 0.67 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 7 | 0.67 |
| (1,190) | 1:10:A:PHE:HD2 | 1:5:A:ASN:HD22 | 18 | 0.67 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 10 | 0.67 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 14 | 0.67 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 12 | 0.67 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 15 | 0.67 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 16 | 0.67 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 7 | 0.66 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 3 | 0.66 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD23 | 15 | 0.66 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 5 | 0.66 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 2 | 0.66 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 6 | 0.66 |
| (1,508) | 1:13:A:PRO:HD2 | 1:12:A:GLY:HA2 | 17 | 0.66 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD11 | 17 | 0.66 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 18 | 0.66 |
| (1,290) | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3 | 6 | 0.66 |
| (1,290) | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3 | 18 | 0.66 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 7 | 0.66 |
| (1,238) | 1:6:A:LEU:HD21 | 1:34:A:ARG:HB3 | 10 | 0.66 |
| (1,183) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HB3 | 8 | 0.66 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 10 | 0.66 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 19 | 0.66 |
| (1,9) | 1:24:A:CYS:H | 1:43:A:CYS:HB2 | 19 | 0.66 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 4 | 0.65 |
| (2,12) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 13 | 0.65 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD22 | 1 | 0.65 |
| (1,351) | 1:30:A:LEU:HD12 | 1:30:A:LEU:HB3 | 5 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 3 | 0.65 |
| (1,290) | 1:9:A:THR:HG22 | 1:11:A:LYS:HD3 | 11 | 0.65 |
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 20 | 0.65 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD21 | 17 | 0.65 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 14 | 0.65 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 4 | 0.65 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 7 | 0.65 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 1 | 0.65 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 5 | 0.65 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 8 | 0.65 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 18 | 0.65 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 20 | 0.65 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 1 | 0.64 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 13 | 0.64 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 3 | 0.64 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 6 | 0.64 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 12 | 0.64 |
| (1,238) | 1:6:A:LEU:HD22 | 1:34:A:ARG:HB3 | 11 | 0.64 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 12 | 0.64 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 1 | 0.64 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 4 | 0.64 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG23 | 9 | 0.64 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 8 | 0.63 |
| (2,12) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 18 | 0.63 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 2 | 0.63 |
| (1,443) | 1:6:A:LEU:HA | 1:6:A:LEU:HD13 | 19 | 0.63 |
| (1,338) | 1:25:A:ARG:HB3 | 1:25:A:ARG:HD2 | 8 | 0.63 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 14 | 0.63 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 18 | 0.63 |
| (1,272) | 1:15:A:ILE:HD12 | 1:17:A:ASP:HB2 | 20 | 0.63 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD11 | 13 | 0.63 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 9 | 0.63 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 15 | 0.63 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 1 | 0.63 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 1 | 0.62 |
| (2,65) | 1:28:A:GLU:H | 1:28:A:GLU:HG2 | 2 | 0.62 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 14 | 0.62 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 18 | 0.62 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 14 | 0.62 |
| (1,485) | 1:36:A:ARG:HB2 | 1:36:A:ARG:HD2 | 9 | 0.62 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 8 | 0.62 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 9 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,338) | 1:25:A:ARG:HB3 | 1:25:A:ARG:HD2 | 16 | 0.62 |
| (1,338) | 1:25:A:ARG:HB3 | 1:25:A:ARG:HD2 | 20 | 0.62 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 15 | 0.62 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 8 | 0.62 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 16 | 0.62 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 8 | 0.62 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD11 | 18 | 0.62 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 13 | 0.62 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG23 | 20 | 0.62 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 8 | 0.62 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 11 | 0.62 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 13 | 0.62 |
| (2,111) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 15 | 0.61 |
| (2,69) | 1:30:A:LEU:HD22 | 1:28:A:GLU:HB2 | 3 | 0.61 |
| (2,32) | 1:30:A:LEU:HD21 | 1:33:A:GLY:H | 3 | 0.61 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD23 | 4 | 0.61 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD22 | 16 | 0.61 |
| (2,12) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 5 | 0.61 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 4 | 0.61 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 14 | 0.61 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 5 | 0.61 |
| (1,485) | 1:36:A:ARG:HB2 | 1:36:A:ARG:HD2 | 7 | 0.61 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 7 | 0.61 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 5 | 0.61 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD11 | 7 | 0.61 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 18 | 0.61 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD23 | 16 | 0.61 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 17 | 0.61 |
| (1,191) | 1:10:A:PHE:HD2 | 1:42:A:TRP:HZ2 | 6 | 0.61 |
| (1,183) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HB3 | 17 | 0.61 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD13 | 3 | 0.61 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 7 | 0.61 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG23 | 9 | 0.61 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG21 | 16 | 0.61 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 18 | 0.61 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG23 | 10 | 0.61 |
| (1,9) | 1:24:A:CYS:H | 1:43:A:CYS:HB2 | 1 | 0.61 |
| (2,98) | 1:32:A:SER:HB2 | 1:34:A:ARG:H | 10 | 0.6 |
| (2,65) | 1:28:A:GLU:H | 1:28:A:GLU:HG3 | 6 | 0.6 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 13 | 0.6 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD22 | 8 | 0.6 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 10 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 11 | 0.6 |
| (1,508) | 1:13:A:PRO:HD2 | 1:12:A:GLY:HA2 | 7 | 0.6 |
| (1,286) | 1:44:A:THR:HG21 | 1:30:A:LEU:HD13 | 10 | 0.6 |
| (1,249) | 1:31:A:LEU:HD12 | 1:44:A:THR:HG23 | 11 | 0.6 |
| (1,238) | 1:6:A:LEU:HD22 | 1:34:A:ARG:HB3 | 1 | 0.6 |
| (1,238) | 1:6:A:LEU:HD22 | 1:34:A:ARG:HB3 | 13 | 0.6 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 4 | 0.6 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 6 | 0.6 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 8 | 0.6 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 19 | 0.6 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 3 | 0.59 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 9 | 0.59 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 5 | 0.59 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 5 | 0.59 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 9 | 0.59 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD23 | 9 | 0.59 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD23 | 12 | 0.59 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD23 | 20 | 0.59 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 4 | 0.59 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 7 | 0.59 |
| (1,286) | 1:44:A:THR:HG23 | 1:30:A:LEU:HD11 | 20 | 0.59 |
| (1,238) | 1:6:A:LEU:HD21 | 1:34:A:ARG:HB3 | 15 | 0.59 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG23 | 12 | 0.59 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG21 | 17 | 0.59 |
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 8 | 0.58 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD21 | 6 | 0.58 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 7 | 0.58 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 7 | 0.58 |
| (1,383) | 1:4:A:GLU:HG2 | 1:5:A:ASN:HD22 | 4 | 0.58 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 16 | 0.58 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 19 | 0.58 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 9 | 0.58 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD13 | 1 | 0.58 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD13 | 2 | 0.58 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD11 | 16 | 0.58 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 19 | 0.58 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 12 | 0.58 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 11 | 0.58 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 18 | 0.57 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 16 | 0.57 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 19 | 0.57 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HB2 | 13 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 6 | 0.57 |
| (2,69) | 1:30:A:LEU:HD23 | 1:28:A:GLU:HB2 | 19 | 0.57 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 9 | 0.57 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD12 | 13 | 0.57 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 18 | 0.57 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 5 | 0.57 |
| (1,455) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HB2 | 18 | 0.57 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 4 | 0.57 |
| (1,183) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HB3 | 4 | 0.57 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD12 | 18 | 0.57 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 20 | 0.57 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 8 | 0.57 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 10 | 0.57 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 7 | 0.57 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 8 | 0.57 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 5 | 0.57 |
| (2,98) | 1:24:A:CYS:HA | 1:26:A:ASN:H | 14 | 0.56 |
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 3 | 0.56 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD22 | 17 | 0.56 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 12 | 0.56 |
| (1,350) | 1:2:A:THR:HG22 | 1:46:A:ARG:HB3 | 3 | 0.56 |
| (1,255) | 1:31:A:LEU:HD12 | 1:4:A:GLU:HB2 | 11 | 0.56 |
| (1,238) | 1:6:A:LEU:HD21 | 1:34:A:ARG:HB3 | 5 | 0.56 |
| (1,238) | 1:6:A:LEU:HD21 | 1:34:A:ARG:HB3 | 12 | 0.56 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 4 | 0.56 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 7 | 0.56 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD13 | 3 | 0.56 |
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 3 | 0.56 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD11 | 13 | 0.56 |
| (1,65) | 1:4:A:GLU:H | 1:3:A:CYS:HB2 | 13 | 0.56 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 3 | 0.56 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 15 | 0.55 |
| (2,69) | 1:30:A:LEU:HD23 | 1:28:A:GLU:HB2 | 16 | 0.55 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE3 | 5 | 0.55 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 12 | 0.55 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 15 | 0.55 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 18 | 0.55 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 12 | 0.55 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 5 | 0.55 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 8 | 0.55 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD23 | 18 | 0.55 |
| (1,178) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB2 | 16 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,178) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB2 | 18 | 0.55 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG23 | 14 | 0.55 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 6 | 0.55 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG22 | 18 | 0.54 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG23 | 19 | 0.54 |
| (2,69) | 1:30:A:LEU:HD22 | 1:28:A:GLU:HB2 | 6 | 0.54 |
| (2,69) | 1:30:A:LEU:HD21 | 1:28:A:GLU:HB2 | 12 | 0.54 |
| (2,69) | 1:30:A:LEU:HD22 | 1:28:A:GLU:HB2 | 14 | 0.54 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD11 | 12 | 0.54 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD11 | 2 | 0.54 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 11 | 0.54 |
| (1,508) | 1:13:A:PRO:HD2 | 1:12:A:GLY:HA2 | 19 | 0.54 |
| (1,489) | 1:30:A:LEU:HD23 | 1:43:A:CYS:HB3 | 12 | 0.54 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 15 | 0.54 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 4 | 0.54 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 1 | 0.54 |
| (1,269) | 1:15:A:ILE:HG22 | 1:15:A:ILE:HG13 | 9 | 0.54 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 20 | 0.54 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD21 | 9 | 0.54 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 1 | 0.54 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 2 | 0.54 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 6 | 0.54 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 10 | 0.54 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 19 | 0.54 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD23 | 20 | 0.54 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD13 | 14 | 0.54 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD12 | 20 | 0.54 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 15 | 0.54 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD12 | 8 | 0.54 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 2 | 0.54 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG23 | 5 | 0.54 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG22 | 7 | 0.54 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 2 | 0.54 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 3 | 0.54 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 19 | 0.54 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 10 | 0.53 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 4 | 0.53 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 5 | 0.53 |
| (2,98) | 1:24:A:CYS:HA | 1:26:A:ASN:H | 11 | 0.53 |
| (2,98) | 1:32:A:SER:HB2 | 1:34:A:ARG:H | 20 | 0.53 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 7 | 0.53 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 2 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,32) | 1:30:A:LEU:HD21 | 1:33:A:GLY:H | 13 | 0.53 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD21 | 18 | 0.53 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 11 | 0.53 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 14 | 0.53 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 20 | 0.53 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD12 | 8 | 0.53 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 7 | 0.53 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 12 | 0.53 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 9 | 0.53 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 16 | 0.53 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD12 | 16 | 0.53 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 17 | 0.53 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG23 | 11 | 0.53 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 19 | 0.52 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 17 | 0.52 |
| (2,69) | 1:30:A:LEU:HD21 | 1:28:A:GLU:HB2 | 4 | 0.52 |
| (2,64) | 1:13:A:PRO:HG2 | 1:12:A:GLY:HA3 | 11 | 0.52 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB2 | 5 | 0.52 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD11 | 1 | 0.52 |
| (2,10) | 1:27:A:ASN:HD22 | 1:25:A:ARG:HA | 14 | 0.52 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 3 | 0.52 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 15 | 0.52 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 8 | 0.52 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 12 | 0.52 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 13 | 0.52 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD22 | 12 | 0.52 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD21 | 18 | 0.52 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 20 | 0.52 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 14 | 0.52 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD13 | 2 | 0.52 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 20 | 0.52 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 11 | 0.52 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG21 | 3 | 0.52 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 17 | 0.52 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 8 | 0.51 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 4 | 0.51 |
| (2,69) | 1:30:A:LEU:HD21 | 1:28:A:GLU:HB2 | 20 | 0.51 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD11 | 7 | 0.51 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 19 | 0.51 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 17 | 0.51 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD13 | 15 | 0.51 |
| (1,178) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB2 | 12 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 6 | 0.51 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 17 | 0.51 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 20 | 0.51 |
| (1,99) | 1:31:A:LEU:H | 1:31:A:LEU:HD21 | 11 | 0.51 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 11 | 0.51 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 5 | 0.51 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 15 | 0.51 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 12 | 0.5 |
| (2,99) | 1:1:A:LYS:HG2 | 1:1:A:LYS:HA | 11 | 0.5 |
| (2,99) | 1:1:A:LYS:HG3 | 1:1:A:LYS:HA | 12 | 0.5 |
| (2,99) | 1:1:A:LYS:HG2 | 1:1:A:LYS:HA | 14 | 0.5 |
| (2,99) | 1:1:A:LYS:HG2 | 1:1:A:LYS:HA | 16 | 0.5 |
| (2,69) | 1:30:A:LEU:HD21 | 1:28:A:GLU:HB2 | 11 | 0.5 |
| (2,66) | 1:1:A:LYS:HB3 | 1:4:A:GLU:H | 5 | 0.5 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 4 | 0.5 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD22 | 19 | 0.5 |
| (2,19) | 1:42:A:TRP:HE3 | 1:11:A:LYS:HD3 | 12 | 0.5 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 9 | 0.5 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 10 | 0.5 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD22 | 4 | 0.5 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 5 | 0.5 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 20 | 0.5 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 4 | 0.5 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 6 | 0.5 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 1 | 0.5 |
| (1,238) | 1:6:A:LEU:HD22 | 1:34:A:ARG:HB3 | 4 | 0.5 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 14 | 0.5 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD11 | 6 | 0.5 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD12 | 4 | 0.5 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD12 | 17 | 0.5 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 14 | 0.5 |
| (1,99) | 1:31:A:LEU:H | 1:31:A:LEU:HD22 | 10 | 0.5 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD12 | 4 | 0.5 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 8 | 0.49 |
| (2,99) | 1:1:A:LYS:HG2 | 1:1:A:LYS:HA | 3 | 0.49 |
| (2,98) | 1:24:A:CYS:HA | 1:26:A:ASN:H | 16 | 0.49 |
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 10 | 0.49 |
| (2,69) | 1:30:A:LEU:HD23 | 1:28:A:GLU:HB2 | 1 | 0.49 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 13 | 0.49 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD12 | 9 | 0.49 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD12 | 18 | 0.49 |
| (1,600) | 1:6:A:LEU:HG | 1:34:A:ARG:HB3 | 16 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 17 | 0.49 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 14 | 0.49 |
| (1,350) | 1:2:A:THR:HG22 | 1:46:A:ARG:HB3 | 7 | 0.49 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 14 | 0.49 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 3 | 0.49 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 10 | 0.49 |
| (1,256) | 1:45:A:ASN:HA | 1:31:A:LEU:HD13 | 2 | 0.49 |
| (1,238) | 1:6:A:LEU:HD23 | 1:34:A:ARG:HB3 | 17 | 0.49 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 13 | 0.49 |
| (1,176) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HD3 | 3 | 0.49 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 1 | 0.49 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD12 | 12 | 0.49 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 13 | 0.49 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 4 | 0.49 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 6 | 0.49 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 9 | 0.49 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 16 | 0.49 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 8 | 0.49 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD11 | 3 | 0.49 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD12 | 5 | 0.48 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD13 | 13 | 0.48 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 15 | 0.48 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 18 | 0.48 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 5 | 0.48 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 18 | 0.48 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD22 | 11 | 0.48 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD11 | 5 | 0.48 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 19 | 0.48 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 17 | 0.48 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD13 | 15 | 0.48 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 3 | 0.48 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 13 | 0.48 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD23 | 15 | 0.48 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 3 | 0.48 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 4 | 0.48 |
| (1,37) | 1:44:A:THR:H | 1:44:A:THR:HG21 | 10 | 0.48 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 10 | 0.48 |
| (2,99) | 1:1:A:LYS:HG3 | 1:1:A:LYS:HA | 9 | 0.47 |
| (2,99) | 1:1:A:LYS:HG3 | 1:1:A:LYS:HA | 20 | 0.47 |
| (2,98) | 1:32:A:SER:HB2 | 1:34:A:ARG:H | 4 | 0.47 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 16 | 0.47 |
| (2,69) | 1:30:A:LEU:HD23 | 1:28:A:GLU:HB2 | 8 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,69) | 1:30:A:LEU:HD21 | 1:28:A:GLU:HB2 | 9 | 0.47 |
| (2,69) | 1:30:A:LEU:HD21 | 1:28:A:GLU:HB2 | 15 | 0.47 |
| (2,32) | 1:30:A:LEU:HD22 | 1:33:A:GLY:H | 8 | 0.47 |
| (2,32) | 1:30:A:LEU:HD23 | 1:33:A:GLY:H | 11 | 0.47 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD22 | 7 | 0.47 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 4 | 0.47 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 3 | 0.47 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 3 | 0.47 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 16 | 0.47 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 19 | 0.47 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 14 | 0.47 |
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 16 | 0.47 |
| (1,269) | 1:15:A:ILE:HG22 | 1:15:A:ILE:HG13 | 19 | 0.47 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD22 | 2 | 0.47 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 15 | 0.47 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 9 | 0.47 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 13 | 0.47 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 16 | 0.47 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 19 | 0.47 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 20 | 0.47 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD13 | 1 | 0.47 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD13 | 14 | 0.47 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 18 | 0.47 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 12 | 0.47 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 9 | 0.47 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 14 | 0.47 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 19 | 0.47 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 15 | 0.47 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 1 | 0.46 |
| (2,99) | 1:1:A:LYS:HG3 | 1:1:A:LYS:HA | 2 | 0.46 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 14 | 0.46 |
| (2,64) | 1:28:A:GLU:HG2 | 1:24:A:CYS:HA | 1 | 0.46 |
| (2,37) | 1:32:A:SER:HA | 1:25:A:ARG:HG3 | 7 | 0.46 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE2 | 14 | 0.46 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 3 | 0.46 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 7 | 0.46 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 15 | 0.46 |
| (1,275) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HB2 | 19 | 0.46 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 1 | 0.46 |
| (1,237) | 1:6:A:LEU:H | 1:6:A:LEU:HD21 | 3 | 0.46 |
| (1,215) | 1:2:A:THR:HA | 1:31:A:LEU:HD11 | 9 | 0.46 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 10 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 12 | 0.46 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 15 | 0.46 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 18 | 0.46 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 14 | 0.46 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD11 | 20 | 0.46 |
| (1,92) | 1:12:A:GLY:H | 1:11:A:LYS:HA | 17 | 0.46 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 6 | 0.45 |
| (2,111) | 1:28:A:GLU:HG3 | 1:29:A:HIS:HB3 | 18 | 0.45 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 20 | 0.45 |
| (2,99) | 1:1:A:LYS:HG2 | 1:1:A:LYS:HA | 1 | 0.45 |
| (2,99) | 1:1:A:LYS:HG3 | 1:1:A:LYS:HA | 6 | 0.45 |
| (2,99) | 1:1:A:LYS:HG3 | 1:1:A:LYS:HA | 7 | 0.45 |
| (2,99) | 1:1:A:LYS:HG3 | 1:1:A:LYS:HA | 15 | 0.45 |
| (2,32) | 1:30:A:LEU:HD23 | 1:33:A:GLY:H | 9 | 0.45 |
| (2,32) | 1:30:A:LEU:HD22 | 1:33:A:GLY:H | 17 | 0.45 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 2 | 0.45 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 18 | 0.45 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 10 | 0.45 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 6 | 0.45 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 16 | 0.45 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 5 | 0.45 |
| (1,257) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA | 17 | 0.45 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 4 | 0.45 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 7 | 0.45 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 8 | 0.45 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 11 | 0.45 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 18 | 0.45 |
| (1,140) | 1:32:A:SER:H | 1:44:A:THR:HG22 | 3 | 0.45 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 5 | 0.45 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 8 | 0.45 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD23 | 19 | 0.45 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 19 | 0.45 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 7 | 0.45 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 6 | 0.45 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG21 | 14 | 0.45 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 4 | 0.44 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 8 | 0.44 |
| (2,69) | 1:30:A:LEU:HD22 | 1:28:A:GLU:HB2 | 13 | 0.44 |
| (2,32) | 1:30:A:LEU:HD21 | 1:33:A:GLY:H | 18 | 0.44 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 7 | 0.44 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 10 | 0.44 |
| (1,508) | 1:13:A:PRO:HD2 | 1:12:A:GLY:HA2 | 16 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 9 | 0.44 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 6 | 0.44 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 7 | 0.44 |
| (1,282) | 1:30:A:LEU:HD11 | 1:43:A:CYS:HB3 | 9 | 0.44 |
| (1,275) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HB2 | 1 | 0.44 |
| (1,275) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HB2 | 11 | 0.44 |
| (1,269) | 1:15:A:ILE:HG22 | 1:15:A:ILE:HG13 | 20 | 0.44 |
| (1,191) | 1:10:A:PHE:HD2 | 1:42:A:TRP:HZ2 | 18 | 0.44 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 18 | 0.44 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 3 | 0.44 |
| (1,147) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HB3 | 14 | 0.44 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD12 | 7 | 0.44 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD12 | 8 | 0.44 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD11 | 16 | 0.44 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD23 | 7 | 0.44 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 19 | 0.44 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 1 | 0.44 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 11 | 0.44 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 12 | 0.44 |
| (1,21) | 1:3:A:CYS:H | 1:44:A:THR:HG22 | 20 | 0.44 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 12 | 0.43 |
| (2,32) | 1:30:A:LEU:HD21 | 1:33:A:GLY:H | 10 | 0.43 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD13 | 10 | 0.43 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 3 | 0.43 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 5 | 0.43 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 2 | 0.43 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 19 | 0.43 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 13 | 0.43 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 17 | 0.43 |
| (1,288) | 1:44:A:THR:HG22 | 1:31:A:LEU:HB3 | 16 | 0.43 |
| (1,282) | 1:30:A:LEU:HD13 | 1:43:A:CYS:HB3 | 16 | 0.43 |
| (1,275) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HB2 | 7 | 0.43 |
| (1,275) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HB2 | 17 | 0.43 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 14 | 0.43 |
| (1,257) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA | 5 | 0.43 |
| (1,257) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA | 19 | 0.43 |
| (1,257) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA | 20 | 0.43 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD12 | 19 | 0.43 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD22 | 13 | 0.43 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 6 | 0.43 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 3 | 0.43 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 12 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 10 | 0.42 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 11 | 0.42 |
| (2,90) | 1:25:A:ARG:HD2 | 1:30:A:LEU:HD13 | 16 | 0.42 |
| (2,69) | 1:30:A:LEU:HD22 | 1:28:A:GLU:HB2 | 10 | 0.42 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 15 | 0.42 |
| (1,565) | 1:7:A:SER:H | 1:6:A:LEU:HD12 | 10 | 0.42 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 8 | 0.42 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 20 | 0.42 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 4 | 0.42 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 9 | 0.42 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 6 | 0.42 |
| (1,282) | 1:30:A:LEU:HD11 | 1:43:A:CYS:HB3 | 6 | 0.42 |
| (1,282) | 1:30:A:LEU:HD13 | 1:43:A:CYS:HB3 | 18 | 0.42 |
| (1,275) | 1:30:A:LEU:HD23 | 1:30:A:LEU:HB2 | 3 | 0.42 |
| (1,275) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HB2 | 12 | 0.42 |
| (1,275) | 1:30:A:LEU:HD23 | 1:30:A:LEU:HB2 | 13 | 0.42 |
| (1,275) | 1:30:A:LEU:HD23 | 1:30:A:LEU:HB2 | 14 | 0.42 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD22 | 2 | 0.42 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 5 | 0.42 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 17 | 0.42 |
| (2,99) | 1:1:A:LYS:HG2 | 1:1:A:LYS:HA | 17 | 0.41 |
| (2,98) | 1:32:A:SER:HB2 | 1:34:A:ARG:H | 12 | 0.41 |
| (2,91) | 1:29:A:HIS:HB3 | 1:28:A:GLU:HG2 | 18 | 0.41 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 3 | 0.41 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 14 | 0.41 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD22 | 1 | 0.41 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD21 | 13 | 0.41 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 6 | 0.41 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 20 | 0.41 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD13 | 4 | 0.41 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD11 | 14 | 0.41 |
| (1,600) | 1:6:A:LEU:HG | 1:34:A:ARG:HB3 | 2 | 0.41 |
| (1,495) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HA | 12 | 0.41 |
| (1,492) | 1:20:A:CYS:HB3 | 1:35:A:CYS:HB2 | 9 | 0.41 |
| (1,472) | 1:36:A:ARG:HB3 | 1:36:A:ARG:HD2 | 2 | 0.41 |
| (1,472) | 1:36:A:ARG:HB3 | 1:36:A:ARG:HD2 | 15 | 0.41 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD23 | 8 | 0.41 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 12 | 0.41 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 6 | 0.41 |
| (1,350) | 1:2:A:THR:HG23 | 1:46:A:ARG:HB3 | 17 | 0.41 |
| (1,288) | 1:44:A:THR:HG21 | 1:31:A:LEU:HB3 | 14 | 0.41 |
| (1,282) | 1:30:A:LEU:HD12 | 1:43:A:CYS:HB3 | 15 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 15 | 0.41 |
| (1,275) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HB2 | 8 | 0.41 |
| (1,275) | 1:30:A:LEU:HD23 | 1:30:A:LEU:HB2 | 10 | 0.41 |
| (1,275) | 1:30:A:LEU:HD23 | 1:30:A:LEU:HB2 | 18 | 0.41 |
| (1,275) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HB2 | 20 | 0.41 |
| (1,269) | 1:15:A:ILE:HG23 | 1:15:A:ILE:HG13 | 16 | 0.41 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 4 | 0.41 |
| (1,138) | 1:32:A:SER:H | 1:31:A:LEU:HD12 | 20 | 0.41 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD11 | 7 | 0.41 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 19 | 0.41 |
| (2,93) | 1:7:A:SER:HB3 | 1:37:A:ASP:HA | 5 | 0.4 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 2 | 0.4 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 10 | 0.4 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG23 | 17 | 0.4 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 8 | 0.4 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 15 | 0.4 |
| (1,449) | 1:39:A:PHE:HB3 | 1:36:A:ARG:HG2 | 19 | 0.4 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 9 | 0.4 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD23 | 7 | 0.4 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD23 | 15 | 0.4 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 20 | 0.4 |
| (1,288) | 1:44:A:THR:HG21 | 1:31:A:LEU:HB3 | 12 | 0.4 |
| (1,282) | 1:30:A:LEU:HD11 | 1:43:A:CYS:HB3 | 14 | 0.4 |
| (1,275) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HB2 | 4 | 0.4 |
| (1,275) | 1:30:A:LEU:HD23 | 1:30:A:LEU:HB2 | 6 | 0.4 |
| (1,275) | 1:30:A:LEU:HD21 | 1:30:A:LEU:HB2 | 16 | 0.4 |
| (1,257) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA | 12 | 0.4 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 3 | 0.4 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 5 | 0.4 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 12 | 0.4 |
| (1,95) | 1:31:A:LEU:H | 1:31:A:LEU:HG | 11 | 0.4 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 4 | 0.4 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 6 | 0.4 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 6 | 0.4 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 5 | 0.39 |
| (2,67) | 1:13:A:PRO:HG2 | 1:12:A:GLY:H | 3 | 0.39 |
| (2,34) | 1:45:A:ASN:HD21 | 1:30:A:LEU:HB2 | 2 | 0.39 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 1 | 0.39 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD11 | 11 | 0.39 |
| (1,600) | 1:6:A:LEU:HG | 1:34:A:ARG:HB3 | 6 | 0.39 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 20 | 0.39 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 3 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 9 | 0.39 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 17 | 0.39 |
| (1,262) | 1:30:A:LEU:HD21 | 1:31:A:LEU:H | 10 | 0.39 |
| (1,257) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA | 15 | 0.39 |
| (1,255) | 1:31:A:LEU:HD11 | 1:4:A:GLU:HB2 | 9 | 0.39 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 17 | 0.39 |
| (1,136) | 1:32:A:SER:H | 1:31:A:LEU:HD21 | 1 | 0.39 |
| (1,116) | 1:25:A:ARG:H | 1:26:A:ASN:HB3 | 8 | 0.39 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD11 | 15 | 0.39 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 17 | 0.39 |
| (1,95) | 1:31:A:LEU:H | 1:31:A:LEU:HG | 10 | 0.39 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 8 | 0.39 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 18 | 0.39 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 17 | 0.38 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB3 | 5 | 0.38 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 13 | 0.38 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 3 | 0.38 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 20 | 0.38 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 3 | 0.38 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 4 | 0.38 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 14 | 0.38 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 8 | 0.38 |
| (1,600) | 1:6:A:LEU:HG | 1:34:A:ARG:HB3 | 8 | 0.38 |
| (1,481) | 1:25:A:ARG:HD2 | 1:43:A:CYS:HB2 | 16 | 0.38 |
| (1,440) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HD21 | 10 | 0.38 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 18 | 0.38 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 16 | 0.38 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 1 | 0.38 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 8 | 0.38 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 18 | 0.38 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD23 | 19 | 0.38 |
| (1,350) | 1:2:A:THR:HG23 | 1:46:A:ARG:HB3 | 8 | 0.38 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 11 | 0.38 |
| (1,288) | 1:44:A:THR:HG22 | 1:31:A:LEU:HB3 | 8 | 0.38 |
| (1,282) | 1:30:A:LEU:HD12 | 1:43:A:CYS:HB3 | 3 | 0.38 |
| (1,275) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HB2 | 15 | 0.38 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 2 | 0.38 |
| (1,269) | 1:15:A:ILE:HG21 | 1:15:A:ILE:HG13 | 11 | 0.38 |
| (1,257) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA | 7 | 0.38 |
| (1,257) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA | 8 | 0.38 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 6 | 0.38 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 9 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 17 | 0.38 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 15 | 0.38 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 5 | 0.38 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 15 | 0.38 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 10 | 0.37 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 4 | 0.37 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 10 | 0.37 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 18 | 0.37 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 8 | 0.37 |
| (1,508) | 1:13:A:PRO:HD2 | 1:12:A:GLY:HA2 | 10 | 0.37 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 17 | 0.37 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 17 | 0.37 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 12 | 0.37 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 13 | 0.37 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 16 | 0.37 |
| (1,350) | 1:2:A:THR:HG23 | 1:46:A:ARG:HB3 | 5 | 0.37 |
| (1,300) | 1:2:A:THR:HG21 | 1:46:A:ARG:HG2 | 15 | 0.37 |
| (1,288) | 1:44:A:THR:HG22 | 1:31:A:LEU:HB3 | 3 | 0.37 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 20 | 0.37 |
| (1,282) | 1:30:A:LEU:HD11 | 1:43:A:CYS:HB3 | 10 | 0.37 |
| (1,282) | 1:30:A:LEU:HD12 | 1:43:A:CYS:HB3 | 13 | 0.37 |
| (1,275) | 1:30:A:LEU:HD22 | 1:30:A:LEU:HB2 | 9 | 0.37 |
| (1,262) | 1:30:A:LEU:HD21 | 1:31:A:LEU:H | 13 | 0.37 |
| (1,259) | 1:2:A:THR:HG23 | 1:1:A:LYS:HA | 19 | 0.37 |
| (1,257) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA | 13 | 0.37 |
| (1,257) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA | 18 | 0.37 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 7 | 0.37 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 16 | 0.37 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 10 | 0.37 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 7 | 0.37 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 8 | 0.37 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 17 | 0.37 |
| (2,113) | 1:31:A:LEU:HG | 1:25:A:ARG:HD2 | 20 | 0.36 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 9 | 0.36 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 17 | 0.36 |
| (2,37) | 1:32:A:SER:HA | 1:25:A:ARG:HG2 | 20 | 0.36 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD11 | 10 | 0.36 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 4 | 0.36 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD21 | 5 | 0.36 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 14 | 0.36 |
| (1,350) | 1:2:A:THR:HG23 | 1:46:A:ARG:HB3 | 15 | 0.36 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 6 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,288) | 1:44:A:THR:HG21 | 1:31:A:LEU:HB3 | 9 | 0.36 |
| (1,257) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA | 14 | 0.36 |
| (1,257) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA | 16 | 0.36 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 2 | 0.36 |
| (1,140) | 1:32:A:SER:H | 1:44:A:THR:HG22 | 17 | 0.36 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 1 | 0.36 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 13 | 0.36 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 13 | 0.35 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 20 | 0.35 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 7 | 0.35 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 11 | 0.35 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 15 | 0.35 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 16 | 0.35 |
| (2,91) | 1:7:A:SER:HB3 | 1:34:A:ARG:HB3 | 17 | 0.35 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 5 | 0.35 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 6 | 0.35 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 9 | 0.35 |
| (2,69) | 1:30:A:LEU:HD23 | 1:28:A:GLU:HB2 | 7 | 0.35 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD22 | 5 | 0.35 |
| (2,20) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HB2 | 13 | 0.35 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 19 | 0.35 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD11 | 1 | 0.35 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 8 | 0.35 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 20 | 0.35 |
| (1,495) | 1:10:A:PHE:HD2 | 1:10:A:PHE:HA | 8 | 0.35 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 18 | 0.35 |
| (1,350) | 1:2:A:THR:HG21 | 1:46:A:ARG:HB3 | 4 | 0.35 |
| (1,300) | 1:2:A:THR:HG22 | 1:46:A:ARG:HG2 | 6 | 0.35 |
| (1,288) | 1:44:A:THR:HG22 | 1:31:A:LEU:HB3 | 18 | 0.35 |
| (1,269) | 1:15:A:ILE:HG22 | 1:15:A:ILE:HG13 | 15 | 0.35 |
| (1,262) | 1:30:A:LEU:HD21 | 1:31:A:LEU:H | 18 | 0.35 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 16 | 0.35 |
| (1,156) | 1:45:A:ASN:HD22 | 1:31:A:LEU:HD21 | 11 | 0.35 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 1 | 0.35 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 18 | 0.35 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD13 | 19 | 0.35 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 2 | 0.35 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 10 | 0.35 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 18 | 0.35 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 12 | 0.34 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 15 | 0.34 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 18 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 20 | 0.34 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 10 | 0.34 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 13 | 0.34 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 17 | 0.34 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 11 | 0.34 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 15 | 0.34 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB2 | 3 | 0.34 |
| (2,32) | 1:30:A:LEU:HD23 | 1:33:A:GLY:H | 4 | 0.34 |
| (2,32) | 1:30:A:LEU:HD21 | 1:33:A:GLY:H | 6 | 0.34 |
| (2,32) | 1:30:A:LEU:HD21 | 1:33:A:GLY:H | 14 | 0.34 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 20 | 0.34 |
| (1,508) | 1:13:A:PRO:HD2 | 1:12:A:GLY:HA2 | 9 | 0.34 |
| (1,495) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HA | 14 | 0.34 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 1 | 0.34 |
| (1,350) | 1:2:A:THR:HG22 | 1:46:A:ARG:HB3 | 10 | 0.34 |
| (1,288) | 1:44:A:THR:HG22 | 1:31:A:LEU:HB3 | 1 | 0.34 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 15 | 0.34 |
| (1,282) | 1:30:A:LEU:HD13 | 1:43:A:CYS:HB3 | 4 | 0.34 |
| (1,272) | 1:15:A:ILE:HD12 | 1:17:A:ASP:HB2 | 18 | 0.34 |
| (1,262) | 1:30:A:LEU:HD22 | 1:31:A:LEU:H | 8 | 0.34 |
| (1,257) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA | 1 | 0.34 |
| (1,257) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HA | 4 | 0.34 |
| (1,229) | 1:36:A:ARG:HA | 1:15:A:ILE:HD11 | 3 | 0.34 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 18 | 0.34 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 19 | 0.34 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG22 | 13 | 0.34 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 10 | 0.33 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 15 | 0.33 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 13 | 0.33 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 17 | 0.33 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 13 | 0.33 |
| (2,66) | 1:1:A:LYS:HB3 | 1:4:A:GLU:H | 10 | 0.33 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 14 | 0.33 |
| (2,32) | 1:30:A:LEU:HD23 | 1:33:A:GLY:H | 15 | 0.33 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 11 | 0.33 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 17 | 0.33 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 8 | 0.33 |
| (1,495) | 1:10:A:PHE:HD1 | 1:10:A:PHE:HA | 4 | 0.33 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 10 | 0.33 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 19 | 0.33 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 8 | 0.33 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 7 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,407) | 1:38:A:ASP:HB3 | 1:38:A:ASP:H | 5 | 0.33 |
| (1,352) | 1:30:A:LEU:HB3 | 1:31:A:LEU:HD22 | 2 | 0.33 |
| (1,350) | 1:2:A:THR:HG23 | 1:46:A:ARG:HB3 | 13 | 0.33 |
| (1,286) | 1:44:A:THR:HG22 | 1:30:A:LEU:HD11 | 1 | 0.33 |
| (1,280) | 1:30:A:LEU:HD11 | 1:28:A:GLU:HB3 | 16 | 0.33 |
| (1,257) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA | 6 | 0.33 |
| (1,183) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HB3 | 19 | 0.33 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 15 | 0.33 |
| (1,98) | 1:31:A:LEU:H | 1:30:A:LEU:HD11 | 1 | 0.33 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 19 | 0.33 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 3 | 0.33 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 18 | 0.32 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 12 | 0.32 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 17 | 0.32 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD2 | 19 | 0.32 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 2 | 0.32 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 13 | 0.32 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 14 | 0.32 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 6 | 0.32 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 9 | 0.32 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 18 | 0.32 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 20 | 0.32 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 1 | 0.32 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 6 | 0.32 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE2 | 13 | 0.32 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 3 | 0.32 |
| (1,300) | 1:2:A:THR:HG21 | 1:46:A:ARG:HG2 | 17 | 0.32 |
| (1,282) | 1:30:A:LEU:HD13 | 1:43:A:CYS:HB3 | 8 | 0.32 |
| (1,262) | 1:30:A:LEU:HD21 | 1:31:A:LEU:H | 3 | 0.32 |
| (1,257) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA | 3 | 0.32 |
| (1,255) | 1:31:A:LEU:HD11 | 1:4:A:GLU:HB2 | 10 | 0.32 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 8 | 0.32 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 6 | 0.32 |
| (1,72) | 1:20:A:CYS:H | 1:21:A:ASN:HB2 | 1 | 0.32 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 10 | 0.32 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 15 | 0.32 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 20 | 0.31 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 9 | 0.31 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 20 | 0.31 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 8 | 0.31 |
| (2,65) | 1:22:A:LYS:HB2 | 1:26:A:ASN:HD22 | 18 | 0.31 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 16 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD13 | 16 | 0.31 |
| (1,622) | 1:36:A:ARG:H | 1:15:A:ILE:HG12 | 3 | 0.31 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 20 | 0.31 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 15 | 0.31 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 20 | 0.31 |
| (1,429) | 1:46:A:ARG:HD2 | 1:45:A:ASN:HB3 | 13 | 0.31 |
| (1,429) | 1:46:A:ARG:HD2 | 1:45:A:ASN:HB3 | 18 | 0.31 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 12 | 0.31 |
| (1,280) | 1:30:A:LEU:HD13 | 1:28:A:GLU:HB3 | 1 | 0.31 |
| (1,280) | 1:30:A:LEU:HD12 | 1:28:A:GLU:HB3 | 9 | 0.31 |
| (1,262) | 1:30:A:LEU:HD23 | 1:31:A:LEU:H | 9 | 0.31 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD23 | 11 | 0.31 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 3 | 0.31 |
| (1,116) | 1:25:A:ARG:H | 1:26:A:ASN:HB3 | 16 | 0.31 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 12 | 0.31 |
| (1,92) | 1:12:A:GLY:H | 1:11:A:LYS:HA | 18 | 0.31 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 5 | 0.31 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 20 | 0.31 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 9 | 0.31 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 4 | 0.3 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 17 | 0.3 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB3 | 3 | 0.3 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 5 | 0.3 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 11 | 0.3 |
| (2,74) | 1:24:A:CYS:HB2 | 1:21:A:ASN:HB2 | 2 | 0.3 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 8 | 0.3 |
| (2,69) | 1:30:A:LEU:HD22 | 1:28:A:GLU:HB2 | 18 | 0.3 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD2 | 8 | 0.3 |
| (2,19) | 1:42:A:TRP:HE3 | 1:11:A:LYS:HD3 | 18 | 0.3 |
| (1,457) | 1:22:A:LYS:HD3 | 1:19:A:ASN:HB3 | 2 | 0.3 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 15 | 0.3 |
| (1,288) | 1:44:A:THR:HG22 | 1:31:A:LEU:HB3 | 4 | 0.3 |
| (1,282) | 1:30:A:LEU:HD11 | 1:43:A:CYS:HB3 | 17 | 0.3 |
| (1,280) | 1:30:A:LEU:HD12 | 1:28:A:GLU:HB3 | 10 | 0.3 |
| (1,262) | 1:30:A:LEU:HD23 | 1:31:A:LEU:H | 4 | 0.3 |
| (1,257) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HA | 9 | 0.3 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 4 | 0.3 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 10 | 0.3 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 17 | 0.3 |
| (1,116) | 1:25:A:ARG:H | 1:26:A:ASN:HB3 | 20 | 0.3 |
| (1,53) | 1:30:A:LEU:H | 1:30:A:LEU:HG | 2 | 0.3 |
| (1,36) | 1:44:A:THR:H | 1:31:A:LEU:HG | 10 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG21 | 7 | 0.3 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG22 | 18 | 0.3 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 18 | 0.29 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 3 | 0.29 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 12 | 0.29 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB3 | 19 | 0.29 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 9 | 0.29 |
| (1,622) | 1:36:A:ARG:H | 1:15:A:ILE:HG12 | 7 | 0.29 |
| (1,598) | 1:46:A:ARG:HG2 | 1:31:A:LEU:HD12 | 5 | 0.29 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 10 | 0.29 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 18 | 0.29 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 2 | 0.29 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 11 | 0.29 |
| (1,280) | 1:30:A:LEU:HD11 | 1:28:A:GLU:HB3 | 4 | 0.29 |
| (1,280) | 1:30:A:LEU:HD12 | 1:28:A:GLU:HB3 | 6 | 0.29 |
| (1,259) | 1:2:A:THR:HG22 | 1:1:A:LYS:HA | 20 | 0.29 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 1 | 0.29 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 3 | 0.29 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 2 | 0.29 |
| (1,36) | 1:44:A:THR:H | 1:31:A:LEU:HG | 11 | 0.29 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG23 | 4 | 0.29 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 6 | 0.29 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 5 | 0.28 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 13 | 0.28 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 16 | 0.28 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 1 | 0.28 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 4 | 0.28 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 10 | 0.28 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 15 | 0.28 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 8 | 0.28 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 14 | 0.28 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 6 | 0.28 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 19 | 0.28 |
| (2,91) | 1:7:A:SER:HB3 | 1:34:A:ARG:HB3 | 7 | 0.28 |
| (2,32) | 1:30:A:LEU:HD22 | 1:33:A:GLY:H | 16 | 0.28 |
| (2,32) | 1:30:A:LEU:HD23 | 1:33:A:GLY:H | 20 | 0.28 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 7 | 0.28 |
| (1,598) | 1:46:A:ARG:HG2 | 1:31:A:LEU:HD13 | 12 | 0.28 |
| (1,580) | 1:5:A:ASN:HD22 | 1:11:A:LYS:HD3 | 19 | 0.28 |
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 18 | 0.28 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 3 | 0.28 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 5 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 6 | 0.28 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 7 | 0.28 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 10 | 0.28 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 12 | 0.28 |
| (1,407) | 1:38:A:ASP:HB3 | 1:38:A:ASP:H | 3 | 0.28 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 16 | 0.28 |
| (1,300) | 1:2:A:THR:HG21 | 1:46:A:ARG:HG2 | 20 | 0.28 |
| (1,282) | 1:30:A:LEU:HD12 | 1:43:A:CYS:HB3 | 20 | 0.28 |
| (1,280) | 1:30:A:LEU:HD11 | 1:28:A:GLU:HB3 | 8 | 0.28 |
| (1,280) | 1:30:A:LEU:HD13 | 1:28:A:GLU:HB3 | 15 | 0.28 |
| (1,262) | 1:30:A:LEU:HD21 | 1:31:A:LEU:H | 14 | 0.28 |
| (1,259) | 1:2:A:THR:HG23 | 1:1:A:LYS:HA | 14 | 0.28 |
| (1,257) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HA | 2 | 0.28 |
| (1,255) | 1:31:A:LEU:HD11 | 1:4:A:GLU:HB2 | 6 | 0.28 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD22 | 10 | 0.28 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD22 | 14 | 0.28 |
| (1,185) | 1:10:A:PHE:HD1 | 1:11:A:LYS:HD3 | 18 | 0.28 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 18 | 0.28 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 8 | 0.28 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD21 | 4 | 0.28 |
| (1,53) | 1:30:A:LEU:H | 1:30:A:LEU:HG | 5 | 0.28 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG22 | 5 | 0.28 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG23 | 16 | 0.28 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 19 | 0.28 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 5 | 0.27 |
| (2,114) | 1:9:A:THR:H | 1:14:A:CYS:HB3 | 19 | 0.27 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD2 | 5 | 0.27 |
| (2,108) | 1:10:A:PHE:H | 1:11:A:LYS:HD3 | 15 | 0.27 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 12 | 0.27 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG22 | 14 | 0.27 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 7 | 0.27 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 6 | 0.27 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD23 | 11 | 0.27 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 7 | 0.27 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 15 | 0.27 |
| (1,614) | 1:29:A:HIS:H | 1:25:A:ARG:HD3 | 12 | 0.27 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 4 | 0.27 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 15 | 0.27 |
| (1,415) | 1:45:A:ASN:HB3 | 1:43:A:CYS:HB3 | 5 | 0.27 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 3 | 0.27 |
| (1,350) | 1:2:A:THR:HG22 | 1:46:A:ARG:HB3 | 2 | 0.27 |
| (1,280) | 1:30:A:LEU:HD11 | 1:28:A:GLU:HB3 | 18 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,259) | 1:2:A:THR:HG22 | 1:1:A:LYS:HA | 17 | 0.27 |
| (1,258) | 1:31:A:LEU:HD12 | 1:44:A:THR:HB | 11 | 0.27 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD23 | 4 | 0.27 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD23 | 5 | 0.27 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD22 | 10 | 0.27 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 11 | 0.27 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 12 | 0.27 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 13 | 0.27 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 19 | 0.27 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 5 | 0.27 |
| (1,143) | 1:32:A:SER:H | 1:31:A:LEU:HG | 10 | 0.27 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 11 | 0.27 |
| (1,92) | 1:12:A:GLY:H | 1:11:A:LYS:HA | 5 | 0.27 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG23 | 12 | 0.27 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 11 | 0.26 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 18 | 0.26 |
| (2,116) | 1:37:A:ASP:HA | 1:38:A:ASP:HB2 | 19 | 0.26 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 9 | 0.26 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 6 | 0.26 |
| (2,32) | 1:30:A:LEU:HD23 | 1:33:A:GLY:H | 12 | 0.26 |
| (2,20) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HB2 | 20 | 0.26 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 20 | 0.26 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD11 | 17 | 0.26 |
| (1,600) | 1:6:A:LEU:HG | 1:34:A:ARG:HB3 | 14 | 0.26 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 5 | 0.26 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 19 | 0.26 |
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 6 | 0.26 |
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 17 | 0.26 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 3 | 0.26 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 1 | 0.26 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 8 | 0.26 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 5 | 0.26 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 2 | 0.26 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 13 | 0.26 |
| (1,288) | 1:44:A:THR:HG22 | 1:31:A:LEU:HB3 | 17 | 0.26 |
| (1,262) | 1:30:A:LEU:HD23 | 1:31:A:LEU:H | 20 | 0.26 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD23 | 12 | 0.26 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 18 | 0.26 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 10 | 0.26 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 12 | 0.26 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 14 | 0.26 |
| (1,156) | 1:45:A:ASN:HD22 | 1:31:A:LEU:HD23 | 10 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 14 | 0.26 |
| (1,143) | 1:32:A:SER:H | 1:31:A:LEU:HG | 11 | 0.26 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 14 | 0.26 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 6 | 0.26 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 15 | 0.25 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 14 | 0.25 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 11 | 0.25 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 4 | 0.25 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 12 | 0.25 |
| (2,56) | 1:28:A:GLU:HG2 | 1:30:A:LEU:HD13 | 15 | 0.25 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB3 | 8 | 0.25 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 3 | 0.25 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD2 | 4 | 0.25 |
| (2,31) | 1:30:A:LEU:HD11 | 1:33:A:GLY:H | 12 | 0.25 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 19 | 0.25 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 16 | 0.25 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 2 | 0.25 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 10 | 0.25 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 8 | 0.25 |
| (1,288) | 1:44:A:THR:HG23 | 1:31:A:LEU:HB3 | 19 | 0.25 |
| (1,280) | 1:30:A:LEU:HD13 | 1:28:A:GLU:HB3 | 7 | 0.25 |
| (1,280) | 1:30:A:LEU:HD12 | 1:28:A:GLU:HB3 | 17 | 0.25 |
| (1,280) | 1:30:A:LEU:HD12 | 1:28:A:GLU:HB3 | 19 | 0.25 |
| (1,262) | 1:30:A:LEU:HD22 | 1:31:A:LEU:H | 7 | 0.25 |
| (1,262) | 1:30:A:LEU:HD23 | 1:31:A:LEU:H | 11 | 0.25 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD21 | 11 | 0.25 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD23 | 16 | 0.25 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 19 | 0.25 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 9 | 0.25 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 20 | 0.25 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 4 | 0.25 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 4 | 0.25 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG21 | 10 | 0.25 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 10 | 0.24 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 8 | 0.24 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 17 | 0.24 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 1 | 0.24 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 4 | 0.24 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 12 | 0.24 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB3 | 18 | 0.24 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 16 | 0.24 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 20 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,600) | 1:6:A:LEU:HG | 1:34:A:ARG:HB3 | 9 | 0.24 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 7 | 0.24 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 11 | 0.24 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 16 | 0.24 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 11 | 0.24 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 16 | 0.24 |
| (1,442) | 1:6:A:LEU:HG | 1:34:A:ARG:HD2 | 6 | 0.24 |
| (1,395) | 1:24:A:CYS:HB3 | 1:21:A:ASN:HA | 17 | 0.24 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 6 | 0.24 |
| (1,282) | 1:30:A:LEU:HD11 | 1:43:A:CYS:HB3 | 11 | 0.24 |
| (1,259) | 1:2:A:THR:HG23 | 1:1:A:LYS:HA | 3 | 0.24 |
| (1,259) | 1:2:A:THR:HG22 | 1:1:A:LYS:HA | 15 | 0.24 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD21 | 2 | 0.24 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD21 | 6 | 0.24 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD22 | 15 | 0.24 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD23 | 17 | 0.24 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD23 | 4 | 0.24 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 1 | 0.24 |
| (1,123) | 1:27:A:ASN:HD22 | 1:26:A:ASN:H | 9 | 0.24 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 3 | 0.24 |
| (2,113) | 1:31:A:LEU:HG | 1:43:A:CYS:HB3 | 7 | 0.23 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 20 | 0.23 |
| (2,108) | 1:10:A:PHE:H | 1:11:A:LYS:HD3 | 3 | 0.23 |
| (2,108) | 1:10:A:PHE:H | 1:11:A:LYS:HD3 | 8 | 0.23 |
| (2,108) | 1:10:A:PHE:H | 1:11:A:LYS:HD3 | 20 | 0.23 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 17 | 0.23 |
| (2,67) | 1:13:A:PRO:HG2 | 1:12:A:GLY:H | 1 | 0.23 |
| (2,67) | 1:13:A:PRO:HG2 | 1:12:A:GLY:H | 16 | 0.23 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 18 | 0.23 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 14 | 0.23 |
| (1,600) | 1:6:A:LEU:HG | 1:34:A:ARG:HB3 | 3 | 0.23 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 2 | 0.23 |
| (1,442) | 1:6:A:LEU:HG | 1:34:A:ARG:HD2 | 9 | 0.23 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 1 | 0.23 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 5 | 0.23 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 17 | 0.23 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 20 | 0.23 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 19 | 0.23 |
| (1,280) | 1:30:A:LEU:HD13 | 1:28:A:GLU:HB3 | 20 | 0.23 |
| (1,262) | 1:30:A:LEU:HD22 | 1:31:A:LEU:H | 16 | 0.23 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD23 | 1 | 0.23 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD23 | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD22 | 7 | 0.23 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD21 | 9 | 0.23 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD21 | 13 | 0.23 |
| (1,248) | 1:31:A:LEU:HD12 | 1:31:A:LEU:HD21 | 18 | 0.23 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 19 | 0.23 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 11 | 0.23 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 20 | 0.23 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 19 | 0.23 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 18 | 0.23 |
| (1,33) | 1:37:A:ASP:H | 1:39:A:PHE:HB3 | 19 | 0.23 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG21 | 2 | 0.23 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG22 | 8 | 0.23 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 1 | 0.22 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 8 | 0.22 |
| (2,97) | 1:8:A:GLY:HA2 | 1:13:A:PRO:HB3 | 8 | 0.22 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 9 | 0.22 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 5 | 0.22 |
| (2,87) | 1:44:A:THR:H | 1:43:A:CYS:HB3 | 15 | 0.22 |
| (2,67) | 1:13:A:PRO:HG2 | 1:12:A:GLY:H | 19 | 0.22 |
| (2,66) | 1:1:A:LYS:HB2 | 1:4:A:GLU:H | 17 | 0.22 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 20 | 0.22 |
| (2,36) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 16 | 0.22 |
| (2,8) | 1:2:A:THR:H | 1:1:A:LYS:HG2 | 13 | 0.22 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD12 | 3 | 0.22 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 15 | 0.22 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 1 | 0.22 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 6 | 0.22 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 9 | 0.22 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 9 | 0.22 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 10 | 0.22 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 18 | 0.22 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 18 | 0.22 |
| (1,350) | 1:2:A:THR:HG23 | 1:46:A:ARG:HB3 | 20 | 0.22 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 14 | 0.22 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD21 | 8 | 0.22 |
| (1,248) | 1:31:A:LEU:HD11 | 1:31:A:LEU:HD21 | 14 | 0.22 |
| (1,248) | 1:31:A:LEU:HD13 | 1:31:A:LEU:HD21 | 20 | 0.22 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD23 | 13 | 0.22 |
| (1,191) | 1:10:A:PHE:HD1 | 1:42:A:TRP:HZ2 | 2 | 0.22 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 6 | 0.22 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 13 | 0.22 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 4 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 7 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 8 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 9 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 10 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 11 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 12 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 13 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 15 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 16 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 17 | 0.22 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 19 | 0.22 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 9 | 0.22 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 17 | 0.22 |
| (1,17) | 1:33:A:GLY:H | 1:32:A:SER:HB3 | 2 | 0.22 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 4 | 0.21 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 2 | 0.21 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 16 | 0.21 |
| (2,98) | 1:32:A:SER:HB2 | 1:34:A:ARG:H | 2 | 0.21 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 1 | 0.21 |
| (2,65) | 1:22:A:LYS:HB2 | 1:26:A:ASN:HD22 | 10 | 0.21 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD2 | 1 | 0.21 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD2 | 12 | 0.21 |
| (2,36) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 20 | 0.21 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 5 | 0.21 |
| (2,8) | 1:2:A:THR:H | 1:1:A:LYS:HG2 | 8 | 0.21 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD11 | 7 | 0.21 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 8 | 0.21 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 13 | 0.21 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 14 | 0.21 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 16 | 0.21 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 18 | 0.21 |
| (1,454) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HA | 13 | 0.21 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 13 | 0.21 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 15 | 0.21 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 20 | 0.21 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 7 | 0.21 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 12 | 0.21 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 2 | 0.21 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 15 | 0.21 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 16 | 0.21 |
| (1,300) | 1:2:A:THR:HG23 | 1:46:A:ARG:HG2 | 9 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,250) | 1:31:A:LEU:HD11 | 1:2:A:THR:HG22 | 19 | 0.21 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 20 | 0.21 |
| (1,191) | 1:10:A:PHE:HD1 | 1:42:A:TRP:HZ2 | 9 | 0.21 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 4 | 0.21 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 20 | 0.21 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 3 | 0.21 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 14 | 0.21 |
| (1,165) | 1:26:A:ASN:HD22 | 1:26:A:ASN:HB3 | 18 | 0.21 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 11 | 0.21 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 12 | 0.21 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD22 | 9 | 0.21 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 2 | 0.2 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 6 | 0.2 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG3 | 16 | 0.2 |
| (2,66) | 1:1:A:LYS:HB2 | 1:4:A:GLU:H | 1 | 0.2 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD2 | 9 | 0.2 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 11 | 0.2 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD2 | 17 | 0.2 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE2 | 7 | 0.2 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD12 | 13 | 0.2 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 8 | 0.2 |
| (1,598) | 1:46:A:ARG:HG2 | 1:31:A:LEU:HD11 | 1 | 0.2 |
| (1,598) | 1:46:A:ARG:HG2 | 1:31:A:LEU:HD11 | 11 | 0.2 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 3 | 0.2 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 10 | 0.2 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 8 | 0.2 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 17 | 0.2 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 8 | 0.2 |
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 12 | 0.2 |
| (1,450) | 1:39:A:PHE:HB3 | 1:20:A:CYS:HB3 | 15 | 0.2 |
| (1,442) | 1:6:A:LEU:HG | 1:34:A:ARG:HD2 | 3 | 0.2 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 5 | 0.2 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 10 | 0.2 |
| (1,229) | 1:36:A:ARG:HA | 1:15:A:ILE:HD11 | 5 | 0.2 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 17 | 0.2 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 3 | 0.2 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 11 | 0.2 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 17 | 0.2 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 18 | 0.2 |
| (1,35) | 1:37:A:ASP:H | 1:36:A:ARG:HB3 | 12 | 0.2 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 5 | 0.19 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 11 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 5 | 0.19 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 13 | 0.19 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG2 | 15 | 0.19 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 7 | 0.19 |
| (2,96) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HA | 8 | 0.19 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 10 | 0.19 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 9 | 0.19 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 10 | 0.19 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 9 | 0.19 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 9 | 0.19 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 20 | 0.19 |
| (1,441) | 1:34:A:ARG:HD3 | 1:6:A:LEU:HG | 8 | 0.19 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 15 | 0.19 |
| (1,364) | 1:34:A:ARG:H | 1:34:A:ARG:HB3 | 2 | 0.19 |
| (1,364) | 1:34:A:ARG:H | 1:34:A:ARG:HB3 | 6 | 0.19 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 3 | 0.19 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 13 | 0.19 |
| (1,242) | 1:11:A:LYS:HD2 | 1:6:A:LEU:HD22 | 6 | 0.19 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 14 | 0.19 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 19 | 0.19 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 17 | 0.19 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 7 | 0.19 |
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 16 | 0.19 |
| (1,140) | 1:32:A:SER:H | 1:44:A:THR:HG21 | 12 | 0.19 |
| (1,116) | 1:25:A:ARG:H | 1:26:A:ASN:HB3 | 10 | 0.19 |
| (1,106) | 1:39:A:PHE:H | 1:36:A:ARG:HB3 | 1 | 0.19 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 10 | 0.19 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 20 | 0.19 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG23 | 11 | 0.19 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 10 | 0.18 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 14 | 0.18 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 16 | 0.18 |
| (2,117) | 1:18:A:GLY:H | 1:36:A:ARG:H | 4 | 0.18 |
| (2,108) | 1:10:A:PHE:H | 1:11:A:LYS:HD3 | 16 | 0.18 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB2 | 6 | 0.18 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB2 | 15 | 0.18 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 15 | 0.18 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 18 | 0.18 |
| (2,4) | 1:44:A:THR:H | 1:30:A:LEU:HD13 | 18 | 0.18 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 6 | 0.18 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 7 | 0.18 |
| (1,594) | 1:21:A:ASN:HD22 | 1:20:A:CYS:HB2 | 12 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 12 | 0.18 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 18 | 0.18 |
| (1,454) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HA | 2 | 0.18 |
| (1,442) | 1:6:A:LEU:HG | 1:34:A:ARG:HD2 | 8 | 0.18 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 6 | 0.18 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 20 | 0.18 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 9 | 0.18 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 13 | 0.18 |
| (1,282) | 1:30:A:LEU:HD11 | 1:43:A:CYS:HB3 | 12 | 0.18 |
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 18 | 0.18 |
| (1,280) | 1:30:A:LEU:HD13 | 1:28:A:GLU:HB3 | 3 | 0.18 |
| (1,255) | 1:31:A:LEU:HD11 | 1:4:A:GLU:HB2 | 16 | 0.18 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 3 | 0.18 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 15 | 0.18 |
| (1,191) | 1:10:A:PHE:HD2 | 1:42:A:TRP:HZ2 | 4 | 0.18 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 8 | 0.18 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD2 | 5 | 0.18 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 1 | 0.18 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 15 | 0.18 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 14 | 0.18 |
| (1,66) | 1:20:A:CYS:H | 1:18:A:GLY:HA3 | 2 | 0.18 |
| (1,33) | 1:37:A:ASP:H | 1:39:A:PHE:HB3 | 3 | 0.18 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 12 | 0.18 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 8 | 0.17 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 17 | 0.17 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 8 | 0.17 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG2 | 19 | 0.17 |
| (2,70) | 1:36:A:ARG:HB3 | 1:15:A:ILE:HG21 | 4 | 0.17 |
| (2,67) | 1:11:A:LYS:HD3 | 1:12:A:GLY:H | 15 | 0.17 |
| (2,66) | 1:1:A:LYS:HB2 | 1:4:A:GLU:H | 6 | 0.17 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB2 | 20 | 0.17 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 4 | 0.17 |
| (2,32) | 1:30:A:LEU:HD22 | 1:33:A:GLY:H | 7 | 0.17 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD12 | 16 | 0.17 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 3 | 0.17 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 15 | 0.17 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 12 | 0.17 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 14 | 0.17 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 19 | 0.17 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 16 | 0.17 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 8 | 0.17 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 15 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 10 | 0.17 |
| (1,371) | 1:15:A:ILE:HB | 1:17:A:ASP:HB2 | 7 | 0.17 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 4 | 0.17 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 11 | 0.17 |
| (1,298) | 1:11:A:LYS:HG3 | 1:11:A:LYS:HD2 | 1 | 0.17 |
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 19 | 0.17 |
| (1,268) | 1:31:A:LEU:HD22 | 1:44:A:THR:H | 10 | 0.17 |
| (1,259) | 1:2:A:THR:HG23 | 1:1:A:LYS:HA | 6 | 0.17 |
| (1,249) | 1:31:A:LEU:HD11 | 1:44:A:THR:HG21 | 9 | 0.17 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 8 | 0.17 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 12 | 0.17 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 4 | 0.17 |
| (1,141) | 1:45:A:ASN:HD21 | 1:30:A:LEU:HB2 | 11 | 0.17 |
| (1,116) | 1:25:A:ARG:H | 1:26:A:ASN:HB3 | 13 | 0.17 |
| (1,100) | 1:31:A:LEU:H | 1:31:A:LEU:HD13 | 2 | 0.17 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 13 | 0.17 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 20 | 0.17 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 3 | 0.17 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 8 | 0.17 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 6 | 0.17 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 15 | 0.17 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 16 | 0.17 |
| (1,20) | 1:3:A:CYS:H | 1:2:A:THR:HG23 | 1 | 0.17 |
| (1,12) | 1:37:A:ASP:H | 1:16:A:PRO:HA | 9 | 0.17 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 1 | 0.16 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 4 | 0.16 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 13 | 0.16 |
| (3,18) | 1:7:A:SER:N | 1:41:A:CYS:O | 17 | 0.16 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 11 | 0.16 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 16 | 0.16 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 18 | 0.16 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD2 | 2 | 0.16 |
| (2,58) | 1:1:A:LYS:HB2 | 1:1:A:LYS:HD2 | 5 | 0.16 |
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB2 | 14 | 0.16 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 13 | 0.16 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 19 | 0.16 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD11 | 3 | 0.16 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE2 | 17 | 0.16 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 12 | 0.16 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 18 | 0.16 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD11 | 15 | 0.16 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,564) | 1:6:A:LEU:HG | 1:42:A:TRP:HZ2 | 3 | 0.16 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 2 | 0.16 |
| (1,529) | 1:33:A:GLY:HA3 | 1:22:A:LYS:HA | 3 | 0.16 |
| (1,502) | 1:7:A:SER:H | 1:7:A:SER:HB3 | 3 | 0.16 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 2 | 0.16 |
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 4 | 0.16 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 6 | 0.16 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 20 | 0.16 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 15 | 0.16 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 16 | 0.16 |
| (1,381) | 1:36:A:ARG:HB3 | 1:40:A:ARG:HA | 19 | 0.16 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 2 | 0.16 |
| (1,300) | 1:2:A:THR:HG22 | 1:46:A:ARG:HG2 | 3 | 0.16 |
| (1,300) | 1:2:A:THR:HG21 | 1:46:A:ARG:HG2 | 12 | 0.16 |
| (1,280) | 1:30:A:LEU:HD12 | 1:28:A:GLU:HB3 | 12 | 0.16 |
| (1,255) | 1:31:A:LEU:HD13 | 1:4:A:GLU:HB2 | 15 | 0.16 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 6 | 0.16 |
| (1,191) | 1:10:A:PHE:HD1 | 1:42:A:TRP:HZ2 | 8 | 0.16 |
| (1,191) | 1:10:A:PHE:HD2 | 1:42:A:TRP:HZ2 | 14 | 0.16 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 19 | 0.16 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 2 | 0.16 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 4 | 0.16 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 11 | 0.16 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 14 | 0.16 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 4 | 0.16 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 1 | 0.16 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 8 | 0.16 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 9 | 0.16 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 17 | 0.16 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 18 | 0.16 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 19 | 0.16 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 3 | 0.15 |
| (3,20) | 1:32:A:SER:N | 1:44:A:THR:O | 10 | 0.15 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 1 | 0.15 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 2 | 0.15 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 3 | 0.15 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 20 | 0.15 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 10 | 0.15 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 3 | 0.15 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 6 | 0.15 |
| (2,78) | 1:38:A:ASP:HB3 | 1:18:A:GLY:HA2 | 5 | 0.15 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 15 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,48) | 1:31:A:LEU:HB2 | 1:1:A:LYS:HB3 | 4 | 0.15 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 20 | 0.15 |
| (2,33) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 7 | 0.15 |
| (2,20) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HG3 | 7 | 0.15 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 15 | 0.15 |
| (2,5) | 1:26:A:ASN:H | 1:29:A:HIS:HA | 16 | 0.15 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 20 | 0.15 |
| (1,613) | 1:25:A:ARG:HD3 | 1:29:A:HIS:HE1 | 16 | 0.15 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 6 | 0.15 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 8 | 0.15 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 9 | 0.15 |
| (1,556) | 1:36:A:ARG:H | 1:39:A:PHE:HB3 | 1 | 0.15 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 2 | 0.15 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 5 | 0.15 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 11 | 0.15 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 13 | 0.15 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 16 | 0.15 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 6 | 0.15 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 13 | 0.15 |
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 8 | 0.15 |
| (1,454) | 1:22:A:LYS:HE2 | 1:19:A:ASN:HA | 19 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 1 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 4 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 5 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 7 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 8 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 9 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 12 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 15 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 16 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 17 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 18 | 0.15 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 19 | 0.15 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 7 | 0.15 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 4 | 0.15 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 9 | 0.15 |
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 8 | 0.15 |
| (1,258) | 1:31:A:LEU:HD11 | 1:44:A:THR:HB | 9 | 0.15 |
| (1,250) | 1:31:A:LEU:HD11 | 1:2:A:THR:HG21 | 17 | 0.15 |
| (1,250) | 1:31:A:LEU:HD13 | 1:2:A:THR:HG21 | 20 | 0.15 |
| (1,218) | 1:2:A:THR:HA | 1:2:A:THR:HB | 9 | 0.15 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 13 | 0.15 |
| (1,148) | 1:32:A:SER:H | 1:24:A:CYS:HB2 | 18 | 0.15 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD21 | 14 | 0.15 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 9 | 0.15 |
| (1,112) | 1:10:A:PHE:H | 1:11:A:LYS:HB3 | 4 | 0.15 |
| (1,92) | 1:12:A:GLY:H | 1:11:A:LYS:HA | 12 | 0.15 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 9 | 0.15 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 5 | 0.15 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 7 | 0.15 |
| (1,19) | 1:44:A:THR:H | 1:31:A:LEU:HD11 | 9 | 0.15 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 2 | 0.15 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 7 | 0.14 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 9 | 0.14 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 12 | 0.14 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 3 | 0.14 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 12 | 0.14 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 17 | 0.14 |
| (3,1) | 1:24:A:CYS:H | 1:20:A:CYS:O | 16 | 0.14 |
| (2,107) | 1:45:A:ASN:HD22 | 1:28:A:GLU:HG2 | 11 | 0.14 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 18 | 0.14 |
| (2,93) | 1:7:A:SER:HB3 | 1:40:A:ARG:HA | 1 | 0.14 |
| (2,65) | 1:22:A:LYS:HB2 | 1:26:A:ASN:HD22 | 15 | 0.14 |
| (2,51) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HD3 | 2 | 0.14 |
| (2,28) | 1:45:A:ASN:HA | 1:30:A:LEU:HD13 | 14 | 0.14 |
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE3 | 8 | 0.14 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 17 | 0.14 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 17 | 0.14 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 5 | 0.14 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 15 | 0.14 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 14 | 0.14 |
| (1,568) | 1:22:A:LYS:HG2 | 1:22:A:LYS:H | 2 | 0.14 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 6 | 0.14 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 13 | 0.14 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 5 | 0.14 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 17 | 0.14 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 18 | 0.14 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 10 | 0.14 |
| (1,492) | 1:20:A:CYS:HB3 | 1:35:A:CYS:HB2 | 3 | 0.14 |
| (1,482) | 1:36:A:ARG:HD3 | 1:39:A:PHE:HB3 | 20 | 0.14 |
| (1,479) | 1:36:A:ARG:HD3 | 1:40:A:ARG:HA | 20 | 0.14 |
| (1,450) | 1:39:A:PHE:HB3 | 1:20:A:CYS:HB3 | 5 | 0.14 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 11 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,432) | 1:46:A:ARG:HB3 | 1:46:A:ARG:HD2 | 1 | 0.14 |
| (1,429) | 1:46:A:ARG:HD2 | 1:45:A:ASN:HB3 | 7 | 0.14 |
| (1,412) | 1:36:A:ARG:HG3 | 1:20:A:CYS:HB3 | 13 | 0.14 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 12 | 0.14 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 12 | 0.14 |
| (1,379) | 1:36:A:ARG:HB3 | 1:39:A:PHE:HB3 | 7 | 0.14 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 7 | 0.14 |
| (1,357) | 1:28:A:GLU:HG2 | 1:28:A:GLU:HA | 14 | 0.14 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 17 | 0.14 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 8 | 0.14 |
| (1,316) | 1:25:A:ARG:HB2 | 1:25:A:ARG:HD3 | 12 | 0.14 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 12 | 0.14 |
| (1,300) | 1:2:A:THR:HG21 | 1:46:A:ARG:HG2 | 1 | 0.14 |
| (1,298) | 1:11:A:LYS:HG3 | 1:11:A:LYS:HD2 | 4 | 0.14 |
| (1,280) | 1:30:A:LEU:HD13 | 1:28:A:GLU:HB3 | 13 | 0.14 |
| (1,262) | 1:30:A:LEU:HD23 | 1:31:A:LEU:H | 12 | 0.14 |
| (1,255) | 1:31:A:LEU:HD12 | 1:4:A:GLU:HB2 | 12 | 0.14 |
| (1,255) | 1:31:A:LEU:HD13 | 1:4:A:GLU:HB2 | 14 | 0.14 |
| (1,191) | 1:10:A:PHE:HD2 | 1:42:A:TRP:HZ2 | 12 | 0.14 |
| (1,176) | 1:39:A:PHE:HD2 | 1:36:A:ARG:HD3 | 2 | 0.14 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 15 | 0.14 |
| (1,167) | 1:19:A:ASN:HD22 | 1:39:A:PHE:HD1 | 16 | 0.14 |
| (1,164) | 1:28:A:GLU:H | 1:27:A:ASN:HB2 | 1 | 0.14 |
| (1,141) | 1:45:A:ASN:HD21 | 1:30:A:LEU:HB2 | 14 | 0.14 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 5 | 0.14 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 7 | 0.14 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 1 | 0.14 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 4 | 0.14 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 4 | 0.14 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 3 | 0.14 |
| (3,20) | 1:32:A:SER:N | 1:44:A:THR:O | 5 | 0.13 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 6 | 0.13 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 9 | 0.13 |
| (3,1) | 1:24:A:CYS:H | 1:20:A:CYS:O | 1 | 0.13 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 14 | 0.13 |
| (2,97) | 1:8:A:GLY:HA2 | 1:13:A:PRO:HB3 | 9 | 0.13 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 1 | 0.13 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 13 | 0.13 |
| (2,66) | 1:1:A:LYS:HB2 | 1:4:A:GLU:H | 9 | 0.13 |
| (2,33) | 1:36:A:ARG:HG2 | 1:20:A:CYS:HB3 | 9 | 0.13 |
| (1,586) | 1:22:A:LYS:HA | 1:25:A:ARG:HB3 | 10 | 0.13 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 18 | 0.13 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 11 | 0.13 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 15 | 0.13 |
| (1,558) | 1:20:A:CYS:HB2 | 1:36:A:ARG:H | 3 | 0.13 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 1 | 0.13 |
| (1,555) | 1:21:A:ASN:H | 1:19:A:ASN:HB3 | 7 | 0.13 |
| (1,525) | 1:28:A:GLU:HB3 | 1:24:A:CYS:HA | 7 | 0.13 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 3 | 0.13 |
| (1,494) | 1:13:A:PRO:HD3 | 1:12:A:GLY:HA3 | 5 | 0.13 |
| (1,475) | 1:36:A:ARG:HD2 | 1:40:A:ARG:HA | 2 | 0.13 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 20 | 0.13 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 10 | 0.13 |
| (1,436) | 1:3:A:CYS:HA | 1:3:A:CYS:HB2 | 13 | 0.13 |
| (1,412) | 1:36:A:ARG:HG3 | 1:20:A:CYS:HB3 | 20 | 0.13 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 17 | 0.13 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 19 | 0.13 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 1 | 0.13 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 11 | 0.13 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 15 | 0.13 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 17 | 0.13 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 18 | 0.13 |
| (1,364) | 1:34:A:ARG:H | 1:34:A:ARG:HB3 | 8 | 0.13 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 20 | 0.13 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 4 | 0.13 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 14 | 0.13 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 17 | 0.13 |
| (1,272) | 1:15:A:ILE:HD13 | 1:17:A:ASP:HB2 | 7 | 0.13 |
| (1,262) | 1:30:A:LEU:HD21 | 1:31:A:LEU:H | 6 | 0.13 |
| (1,249) | 1:31:A:LEU:HD11 | 1:44:A:THR:HG23 | 6 | 0.13 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 6 | 0.13 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 7 | 0.13 |
| (1,164) | 1:28:A:GLU:H | 1:27:A:ASN:HB2 | 11 | 0.13 |
| (1,164) | 1:28:A:GLU:H | 1:27:A:ASN:HB2 | 19 | 0.13 |
| (1,140) | 1:32:A:SER:H | 1:44:A:THR:HG23 | 7 | 0.13 |
| (1,89) | 1:6:A:LEU:H | 1:5:A:ASN:HD22 | 8 | 0.13 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 5 | 0.13 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 13 | 0.13 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 20 | 0.13 |
| (1,68) | 1:20:A:CYS:H | 1:35:A:CYS:HA | 13 | 0.13 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 17 | 0.13 |
| (1,45) | 1:26:A:ASN:H | 1:22:A:LYS:HG2 | 19 | 0.13 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 13 | 0.13 |
| (1,5) | 1:45:A:ASN:H | 1:47:A:CYS:HB2 | 14 | 0.13 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 6 | 0.12 |
| (3,21) | 1:34:A:ARG:H | 1:42:A:TRP:O | 9 | 0.12 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 18 | 0.12 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 19 | 0.12 |
| (3,18) | 1:7:A:SER:N | 1:41:A:CYS:O | 1 | 0.12 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 1 | 0.12 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 14 | 0.12 |
| (3,9) | 1:3:A:CYS:H | 1:45:A:ASN:O | 20 | 0.12 |
| (2,109) | 1:22:A:LYS:HA | 1:22:A:LYS:HD3 | 7 | 0.12 |
| (2,106) | 1:36:A:ARG:H | 1:34:A:ARG:HG2 | 19 | 0.12 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 14 | 0.12 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 16 | 0.12 |
| (2,34) | 1:30:A:LEU:HB2 | 1:32:A:SER:H | 14 | 0.12 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 7 | 0.12 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 16 | 0.12 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD11 | 14 | 0.12 |
| (2,8) | 1:2:A:THR:H | 1:1:A:LYS:HG2 | 19 | 0.12 |
| (2,3) | 1:33:A:GLY:H | 1:45:A:ASN:HA | 11 | 0.12 |
| (2,3) | 1:33:A:GLY:H | 1:45:A:ASN:HA | 12 | 0.12 |
| (1,622) | 1:36:A:ARG:H | 1:15:A:ILE:HG12 | 5 | 0.12 |
| (1,598) | 1:46:A:ARG:HG2 | 1:31:A:LEU:HD12 | 16 | 0.12 |
| (1,586) | 1:22:A:LYS:HA | 1:25:A:ARG:HB3 | 2 | 0.12 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 12 | 0.12 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 11 | 0.12 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 13 | 0.12 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 5 | 0.12 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 7 | 0.12 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 14 | 0.12 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 15 | 0.12 |
| (1,529) | 1:33:A:GLY:HA3 | 1:22:A:LYS:HA | 15 | 0.12 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 6 | 0.12 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 12 | 0.12 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 19 | 0.12 |
| (1,511) | 1:16:A:PRO:HD3 | 1:15:A:ILE:HB | 20 | 0.12 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 7 | 0.12 |
| (1,450) | 1:39:A:PHE:HB3 | 1:20:A:CYS:HB3 | 2 | 0.12 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 4 | 0.12 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 12 | 0.12 |
| (1,364) | 1:34:A:ARG:H | 1:34:A:ARG:HB3 | 3 | 0.12 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,300) | 1:2:A:THR:HG21 | 1:46:A:ARG:HG2 | 4 | 0.12 |
| (1,281) | 1:6:A:LEU:HB3 | 1:11:A:LYS:HD3 | 6 | 0.12 |
| (1,280) | 1:30:A:LEU:HD12 | 1:28:A:GLU:HB3 | 14 | 0.12 |
| (1,268) | 1:31:A:LEU:HD21 | 1:44:A:THR:H | 11 | 0.12 |
| (1,262) | 1:30:A:LEU:HD23 | 1:31:A:LEU:H | 15 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 1 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 2 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 3 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 5 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 7 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 9 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 10 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 13 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 14 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 17 | 0.12 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 20 | 0.12 |
| (1,179) | 1:5:A:ASN:HD22 | 1:6:A:LEU:HA | 6 | 0.12 |
| (1,164) | 1:28:A:GLU:H | 1:27:A:ASN:HB2 | 17 | 0.12 |
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 4 | 0.12 |
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 6 | 0.12 |
| (1,146) | 1:45:A:ASN:HD21 | 1:45:A:ASN:HB3 | 14 | 0.12 |
| (1,141) | 1:45:A:ASN:HD21 | 1:30:A:LEU:HB2 | 10 | 0.12 |
| (1,141) | 1:45:A:ASN:HD21 | 1:30:A:LEU:HB2 | 13 | 0.12 |
| (1,137) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD22 | 18 | 0.12 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 14 | 0.12 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 6 | 0.12 |
| (1,83) | 1:6:A:LEU:H | 1:5:A:ASN:HB3 | 10 | 0.12 |
| (1,46) | 1:26:A:ASN:H | 1:25:A:ARG:HB3 | 14 | 0.12 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 11 | 0.12 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 8 | 0.12 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 18 | 0.12 |
| (3,22) | 1:34:A:ARG:N | 1:42:A:TRP:O | 12 | 0.11 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 14 | 0.11 |
| (3,19) | 1:32:A:SER:H | 1:44:A:THR:O | 15 | 0.11 |
| (3,18) | 1:7:A:SER:N | 1:41:A:CYS:O | 16 | 0.11 |
| (3,1) | 1:24:A:CYS:H | 1:20:A:CYS:O | 9 | 0.11 |
| (3,1) | 1:24:A:CYS:H | 1:20:A:CYS:O | 19 | 0.11 |
| (2,115) | 1:29:A:HIS:H | 1:33:A:GLY:HA3 | 7 | 0.11 |
| (2,110) | 1:37:A:ASP:HB3 | 1:38:A:ASP:H | 5 | 0.11 |
| (2,51) | 1:22:A:LYS:HG3 | 1:22:A:LYS:HD2 | 5 | 0.11 |
| (2,46) | 1:22:A:LYS:HG2 | 1:22:A:LYS:HD3 | 5 | 0.11 |
| (2,20) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HG3 | 9 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,18) | 1:42:A:TRP:HE3 | 1:1:A:LYS:HE3 | 10 | 0.11 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 3 | 0.11 |
| (2,16) | 1:28:A:GLU:H | 1:29:A:HIS:HB2 | 6 | 0.11 |
| (2,3) | 1:33:A:GLY:H | 1:45:A:ASN:HA | 5 | 0.11 |
| (1,620) | 1:22:A:LYS:HB3 | 1:26:A:ASN:HD22 | 5 | 0.11 |
| (1,618) | 1:21:A:ASN:HD22 | 1:25:A:ARG:HD3 | 5 | 0.11 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 2 | 0.11 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 19 | 0.11 |
| (1,591) | 1:20:A:CYS:HB3 | 1:40:A:ARG:H | 13 | 0.11 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 18 | 0.11 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 2 | 0.11 |
| (1,566) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HG3 | 3 | 0.11 |
| (1,562) | 1:42:A:TRP:HZ2 | 1:6:A:LEU:HD22 | 19 | 0.11 |
| (1,529) | 1:33:A:GLY:HA3 | 1:22:A:LYS:HA | 2 | 0.11 |
| (1,529) | 1:33:A:GLY:HA3 | 1:22:A:LYS:HA | 6 | 0.11 |
| (1,529) | 1:33:A:GLY:HA3 | 1:22:A:LYS:HA | 18 | 0.11 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 4 | 0.11 |
| (1,496) | 1:29:A:HIS:HB3 | 1:29:A:HIS:H | 9 | 0.11 |
| (1,483) | 1:20:A:CYS:HB3 | 1:36:A:ARG:HD3 | 3 | 0.11 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 11 | 0.11 |
| (1,420) | 1:26:A:ASN:HB3 | 1:27:A:ASN:HD22 | 10 | 0.11 |
| (1,412) | 1:36:A:ARG:HG3 | 1:20:A:CYS:HB3 | 5 | 0.11 |
| (1,380) | 1:4:A:GLU:HG3 | 1:32:A:SER:HB2 | 14 | 0.11 |
| (1,380) | 1:4:A:GLU:HG3 | 1:32:A:SER:HB2 | 17 | 0.11 |
| (1,380) | 1:4:A:GLU:HG3 | 1:32:A:SER:HB2 | 20 | 0.11 |
| (1,378) | 1:4:A:GLU:HG3 | 1:5:A:ASN:HB3 | 14 | 0.11 |
| (1,364) | 1:34:A:ARG:H | 1:34:A:ARG:HB3 | 9 | 0.11 |
| (1,359) | 1:16:A:PRO:HG3 | 1:17:A:ASP:HA | 19 | 0.11 |
| (1,350) | 1:2:A:THR:HG23 | 1:46:A:ARG:HB3 | 18 | 0.11 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 1 | 0.11 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 1 | 0.11 |
| (1,319) | 1:22:A:LYS:HG2 | 1:19:A:ASN:H | 17 | 0.11 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 3 | 0.11 |
| (1,229) | 1:36:A:ARG:HA | 1:15:A:ILE:HD11 | 4 | 0.11 |
| (1,191) | 1:10:A:PHE:HD2 | 1:42:A:TRP:HZ2 | 19 | 0.11 |
| (1,188) | 1:19:A:ASN:H | 1:36:A:ARG:HD3 | 7 | 0.11 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 4 | 0.11 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 8 | 0.11 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 11 | 0.11 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 15 | 0.11 |
| (1,180) | 1:5:A:ASN:HD22 | 1:5:A:ASN:HB3 | 19 | 0.11 |
| (1,176) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HD3 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 13 | 0.11 |
| (1,146) | 1:45:A:ASN:HD21 | 1:45:A:ASN:HB3 | 2 | 0.11 |
| (1,146) | 1:45:A:ASN:HD21 | 1:45:A:ASN:HB3 | 3 | 0.11 |
| (1,146) | 1:45:A:ASN:HD21 | 1:45:A:ASN:HB3 | 13 | 0.11 |
| (1,141) | 1:45:A:ASN:HD21 | 1:30:A:LEU:HB2 | 18 | 0.11 |
| (1,140) | 1:32:A:SER:H | 1:44:A:THR:HG21 | 14 | 0.11 |
| (1,122) | 1:27:A:ASN:HD22 | 1:24:A:CYS:H | 4 | 0.11 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 10 | 0.11 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 3 | 0.11 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 14 | 0.11 |
| (1,13) | 1:3:A:CYS:H | 1:2:A:THR:HA | 16 | 0.11 |
| (3,20) | 1:32:A:SER:N | 1:44:A:THR:O | 11 | 0.1 |
| (2,97) | 1:8:A:GLY:HA2 | 1:13:A:PRO:HB3 | 12 | 0.1 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 17 | 0.1 |
| (2,71) | 1:13:A:PRO:HB3 | 1:37:A:ASP:HB2 | 20 | 0.1 |
| (2,12) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 19 | 0.1 |
| (1,616) | 1:44:A:THR:HB | 1:2:A:THR:H | 9 | 0.1 |
| (1,604) | 1:45:A:ASN:HD21 | 1:31:A:LEU:HD13 | 7 | 0.1 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 8 | 0.1 |
| (1,583) | 1:33:A:GLY:HA3 | 1:24:A:CYS:H | 10 | 0.1 |
| (1,571) | 1:19:A:ASN:HD22 | 1:20:A:CYS:HA | 5 | 0.1 |
| (1,568) | 1:22:A:LYS:HG2 | 1:22:A:LYS:H | 3 | 0.1 |
| (1,567) | 1:42:A:TRP:HH2 | 1:11:A:LYS:HD3 | 10 | 0.1 |
| (1,529) | 1:33:A:GLY:HA3 | 1:22:A:LYS:HA | 9 | 0.1 |
| (1,459) | 1:22:A:LYS:HG3 | 1:19:A:ASN:HB3 | 7 | 0.1 |
| (1,432) | 1:46:A:ARG:HB3 | 1:46:A:ARG:HD2 | 16 | 0.1 |
| (1,412) | 1:36:A:ARG:HG3 | 1:20:A:CYS:HB3 | 11 | 0.1 |
| (1,410) | 1:47:A:CYS:HB2 | 1:3:A:CYS:HB3 | 10 | 0.1 |
| (1,396) | 1:24:A:CYS:HB3 | 1:25:A:ARG:HD2 | 14 | 0.1 |
| (1,380) | 1:4:A:GLU:HG3 | 1:32:A:SER:HB2 | 12 | 0.1 |
| (1,378) | 1:4:A:GLU:HG3 | 1:5:A:ASN:HB3 | 12 | 0.1 |
| (1,375) | 1:4:A:GLU:HG3 | 1:34:A:ARG:HB3 | 19 | 0.1 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 4 | 0.1 |
| (1,335) | 1:36:A:ARG:HB2 | 1:15:A:ILE:HG12 | 12 | 0.1 |
| (1,309) | 1:25:A:ARG:HG2 | 1:26:A:ASN:H | 19 | 0.1 |
| (1,259) | 1:2:A:THR:HG21 | 1:1:A:LYS:HA | 9 | 0.1 |
| (1,249) | 1:31:A:LEU:HD11 | 1:44:A:THR:HG21 | 10 | 0.1 |
| (1,176) | 1:39:A:PHE:HD1 | 1:36:A:ARG:HD3 | 4 | 0.1 |
| (1,158) | 1:19:A:ASN:HD22 | 1:36:A:ARG:HD3 | 11 | 0.1 |
| (1,146) | 1:45:A:ASN:HD21 | 1:45:A:ASN:HB3 | 6 | 0.1 |
| (1,127) | 1:26:A:ASN:HD21 | 1:26:A:ASN:HA | 3 | 0.1 |
| (1,92) | 1:12:A:GLY:H | 1:11:A:LYS:HA | 14 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|--------|--------------|----------------|----------|---------------|
| (1,61) | 1:7:A:SER:H | 1:7:A:SER:HB2 | 1 | 0.1 |
| (1,46) | 1:26:A:ASN:H | 1:25:A:ARG:HB3 | 11 | 0.1 |
| (1,33) | 1:37:A:ASP:H | 1:39:A:PHE:HB3 | 9 | 0.1 |
| (1,22) | 1:3:A:CYS:H | 1:3:A:CYS:HB3 | 13 | 0.1 |

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

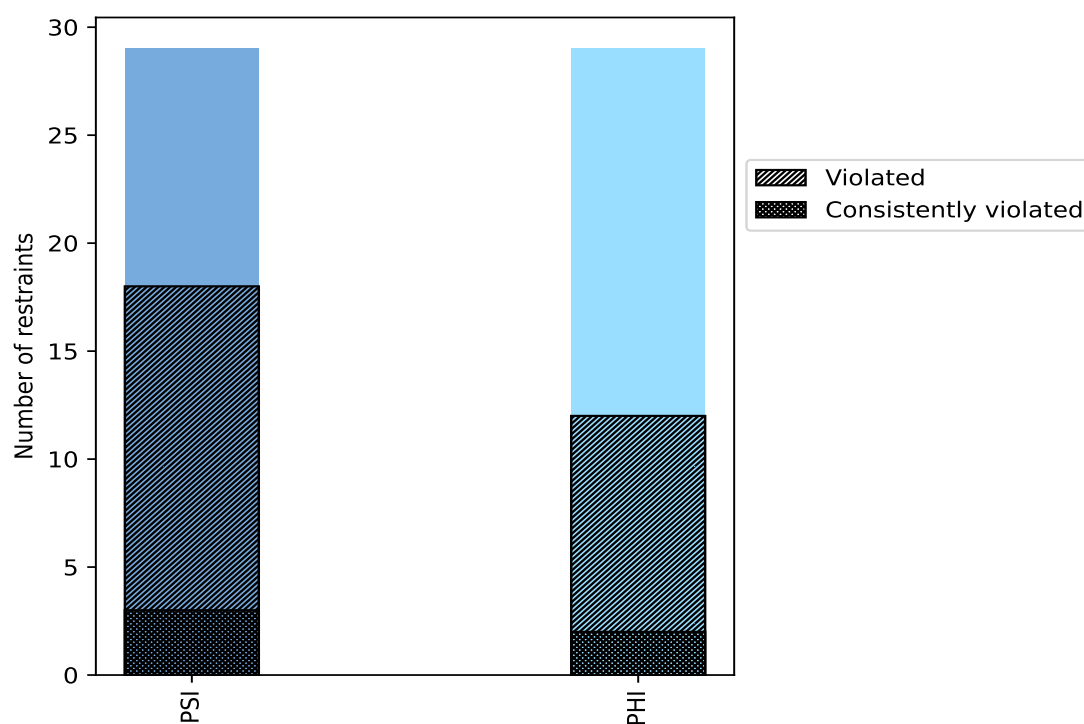
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PSI | 29 | 50.0 | 18 | 62.1 | 31.0 | 3 | 10.3 | 5.2 |
| PHI | 29 | 50.0 | 12 | 41.4 | 20.7 | 2 | 6.9 | 3.4 |
| Total | 58 | 100.0 | 30 | 51.7 | 51.7 | 5 | 8.6 | 8.6 |

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

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



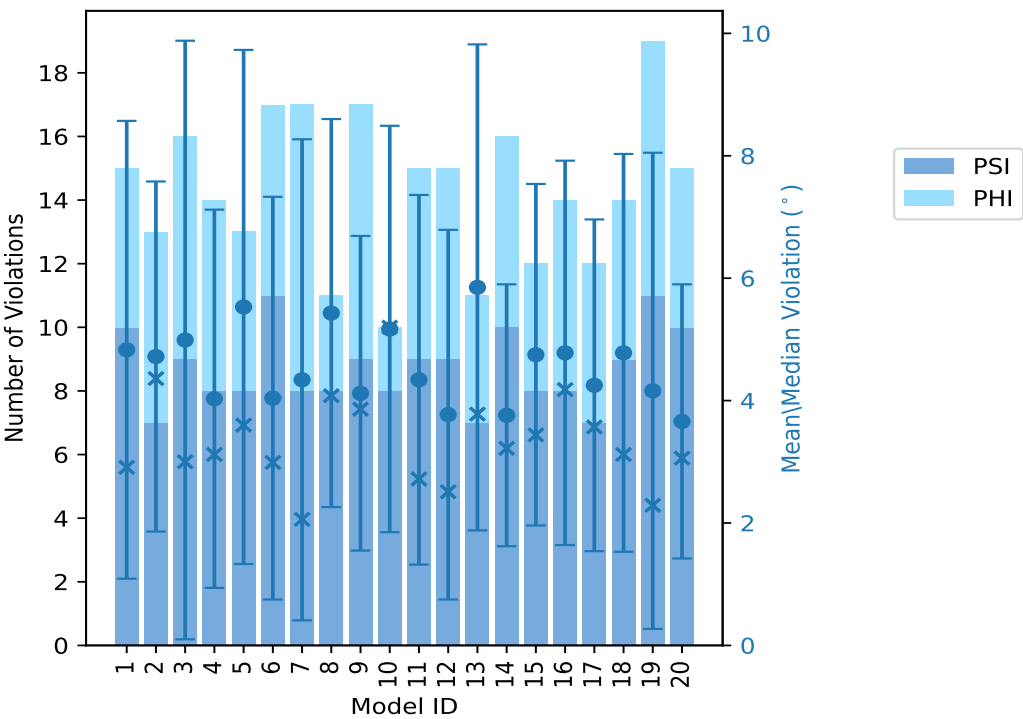
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PSI | PHI | Total | | | | |
| 1 | 10 | 5 | 15 | 4.83 | 12.27 | 3.74 | 2.91 |
| 2 | 7 | 6 | 13 | 4.72 | 9.91 | 2.86 | 4.36 |
| 3 | 9 | 7 | 16 | 4.99 | 17.5 | 4.89 | 3.0 |
| 4 | 8 | 6 | 14 | 4.03 | 10.81 | 3.09 | 3.12 |
| 5 | 8 | 5 | 13 | 5.53 | 13.72 | 4.2 | 3.6 |
| 6 | 11 | 6 | 17 | 4.04 | 11.59 | 3.29 | 2.99 |
| 7 | 8 | 9 | 17 | 4.34 | 12.75 | 3.93 | 2.06 |
| 8 | 8 | 3 | 11 | 5.43 | 11.68 | 3.17 | 4.08 |
| 9 | 9 | 8 | 17 | 4.12 | 10.38 | 2.57 | 3.86 |
| 10 | 8 | 2 | 10 | 5.17 | 10.05 | 3.32 | 5.2 |
| 11 | 9 | 6 | 15 | 4.34 | 10.97 | 3.02 | 2.72 |
| 12 | 9 | 6 | 15 | 3.77 | 10.4 | 3.02 | 2.51 |
| 13 | 7 | 4 | 11 | 5.85 | 13.69 | 3.97 | 3.78 |
| 14 | 10 | 6 | 16 | 3.76 | 9.59 | 2.14 | 3.22 |
| 15 | 8 | 4 | 12 | 4.75 | 10.1 | 2.79 | 3.44 |
| 16 | 8 | 6 | 14 | 4.78 | 12.47 | 3.14 | 4.18 |
| 17 | 7 | 5 | 12 | 4.25 | 9.61 | 2.71 | 3.57 |
| 18 | 9 | 5 | 14 | 4.78 | 10.91 | 3.25 | 3.12 |
| 19 | 11 | 8 | 19 | 4.16 | 13.08 | 3.89 | 2.29 |
| 20 | 10 | 5 | 15 | 3.66 | 9.3 | 2.24 | 3.06 |

10.2.1 Bar graph : Dihedral 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

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

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

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

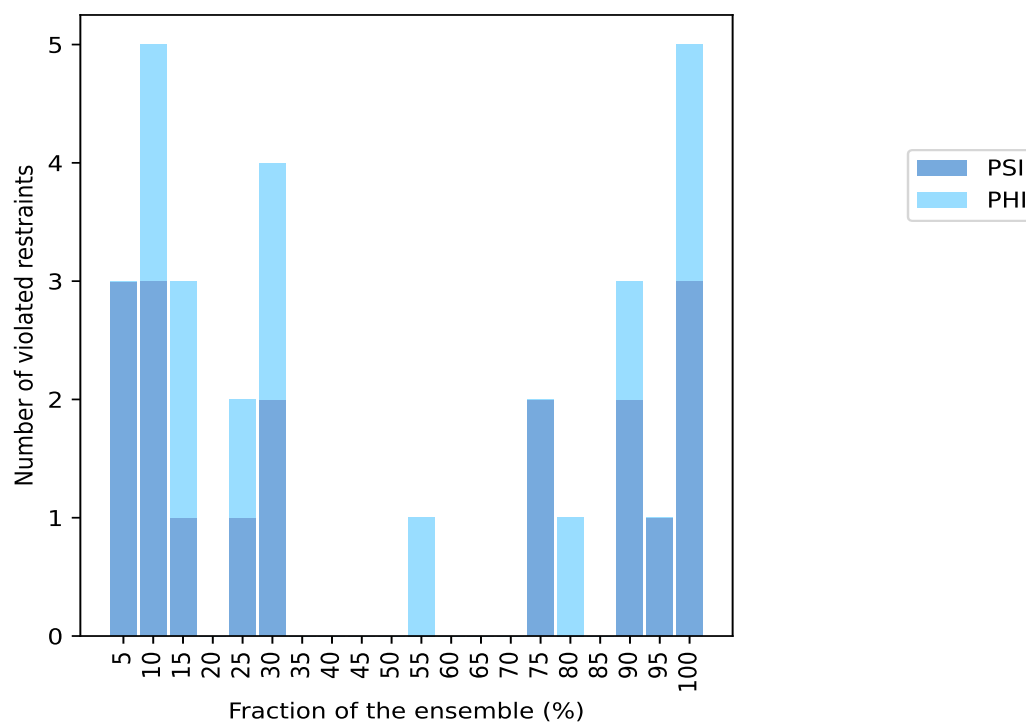
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 60.0 |
| 0 | 0 | 0 | 13 | 65.0 |
| 0 | 0 | 0 | 14 | 70.0 |
| 2 | 0 | 2 | 15 | 75.0 |
| 0 | 1 | 1 | 16 | 80.0 |
| 0 | 0 | 0 | 17 | 85.0 |
| 2 | 1 | 3 | 18 | 90.0 |
| 1 | 0 | 1 | 19 | 95.0 |
| 3 | 2 | 5 | 20 | 100.0 |

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

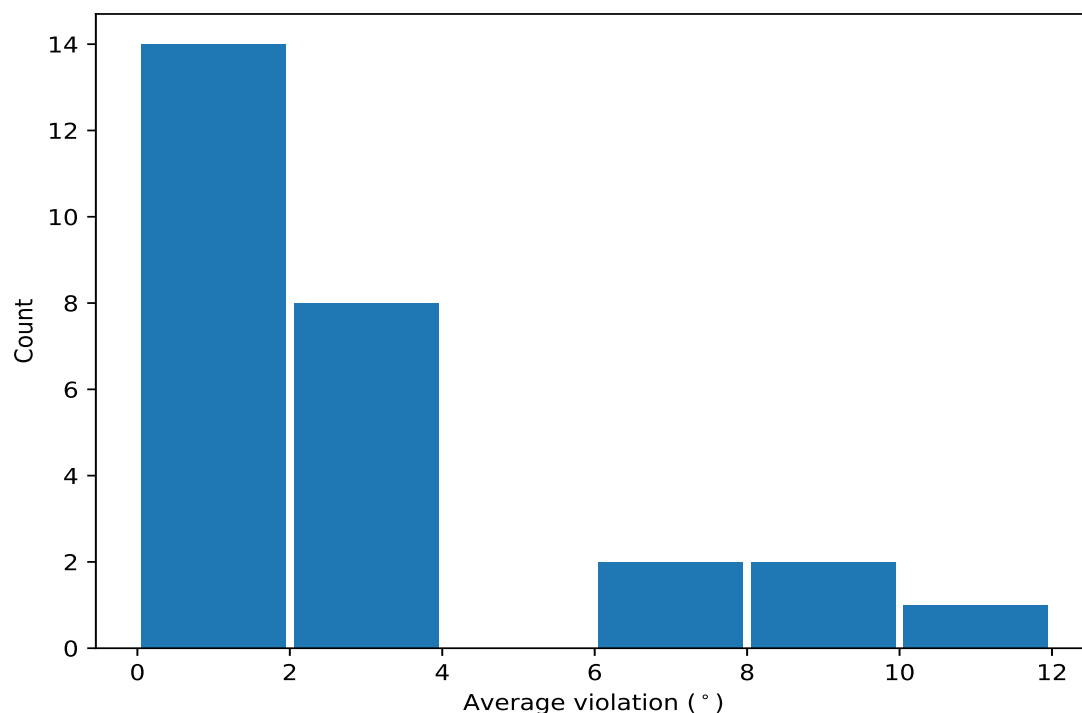


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|-------|-----------------|--------|
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 20 | 11.54 | 1.92 | 10.94 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 20 | 8.4 | 1.62 | 8.38 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 20 | 8.31 | 2.75 | 7.4 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 20 | 6.71 | 2.53 | 7.56 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 20 | 6.43 | 1.72 | 6.53 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 19 | 3.59 | 1.64 | 3.51 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 18 | 3.41 | 1.74 | 3.02 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 18 | 2.95 | 0.9 | 2.87 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 18 | 2.51 | 0.87 | 2.61 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 16 | 3.03 | 1.22 | 2.92 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 15 | 1.99 | 0.66 | 1.93 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 15 | 1.82 | 0.46 | 1.91 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 11 | 1.78 | 0.64 | 1.61 |
| (1,18) | 1:18:A:GLY:N | 1:18:A:GLY:CA | 1:18:A:GLY:C | 1:19:A:ASN:N | 6 | 2.77 | 1.34 | 2.84 |
| (1,42) | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 1:34:A:ARG:N | 6 | 2.15 | 1.11 | 1.72 |
| (1,27) | 1:24:A:CYS:C | 1:25:A:ARG:N | 1:25:A:ARG:CA | 1:25:A:ARG:C | 6 | 1.61 | 0.3 | 1.54 |
| (1,31) | 1:26:A:ASN:C | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 6 | 1.39 | 0.21 | 1.32 |
| (1,9) | 1:5:A:ASN:C | 1:6:A:LEU:N | 1:6:A:LEU:CA | 1:6:A:LEU:C | 5 | 2.66 | 1.23 | 2.47 |
| (1,24) | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C | 1:24:A:CYS:N | 5 | 1.99 | 0.86 | 1.83 |
| (1,41) | 1:32:A:SER:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 3 | 1.64 | 0.27 | 1.48 |

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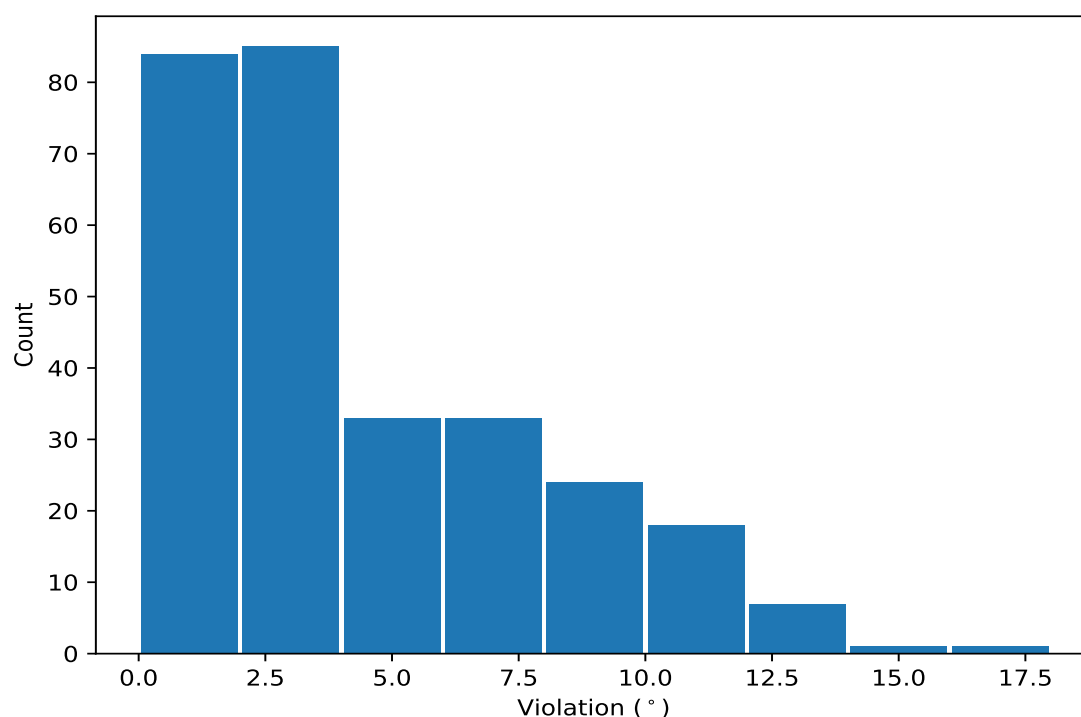
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|--------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,33) | 1:27:A:ASN:C | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 3 | 1.56 | 0.6 | 1.19 |
| (1,32) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:GLU:N | 3 | 1.16 | 0.11 | 1.15 |
| (1,44) | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 1:36:A:ARG:N | 2 | 1.78 | 0.27 | 1.78 |
| (1,14) | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 1:11:A:LYS:N | 2 | 1.66 | 0.57 | 1.66 |
| (1,47) | 1:38:A:ASP:C | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 2 | 1.62 | 0.1 | 1.62 |
| (1,58) | 1:46:A:ARG:N | 1:46:A:ARG:CA | 1:46:A:ARG:C | 1:47:A:CYS:N | 2 | 1.29 | 0.15 | 1.29 |
| (1,11) | 1:6:A:LEU:C | 1:7:A:SER:N | 1:7:A:SER:CA | 1:7:A:SER:C | 2 | 1.23 | 0.02 | 1.23 |

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

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

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

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



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 3 | 17.5 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 3 | 15.46 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 5 | 13.72 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 13 | 13.69 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 19 | 13.08 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 7 | 12.75 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 5 | 12.51 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 16 | 12.47 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 1 | 12.27 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 7 | 11.88 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 8 | 11.68 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 6 | 11.59 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 6 | 11.53 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 11 | 10.97 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 18 | 10.91 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 4 | 10.81 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 1 | 10.81 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 19 | 10.72 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 19 | 10.68 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 12 | 10.4 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 19 | 10.39 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 18 | 10.39 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 9 | 10.38 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 15 | 10.1 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 13 | 10.06 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 10 | 10.05 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 16 | 10.02 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 2 | 9.91 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 5 | 9.89 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 13 | 9.88 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 12 | 9.68 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 17 | 9.61 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 14 | 9.59 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 1 | 9.49 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 1 | 9.39 |
| (1,51) | 1:40:A:ARG:C | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 20 | 9.3 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 15 | 9.29 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 11 | 9.21 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 4 | 9.08 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 10 | 8.89 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 7 | 8.88 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 8 | 8.77 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 7 | 8.57 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 3 | 8.47 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 2 | 8.4 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 10 | 8.38 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 20 | 8.37 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 5 | 8.23 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 6 | 8.05 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 13 | 8.05 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 2 | 8.04 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 18 | 7.97 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 5 | 7.96 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 11 | 7.96 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 17 | 7.95 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 8 | 7.89 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 9 | 7.85 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 18 | 7.7 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 10 | 7.62 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 17 | 7.61 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 4 | 7.57 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 13 | 7.51 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 18 | 7.48 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 3 | 7.42 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 8 | 7.33 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 2 | 7.32 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 8 | 7.27 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 12 | 7.27 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 9 | 7.24 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 7 | 7.24 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 15 | 7.16 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 16 | 7.12 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 11 | 6.92 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 15 | 6.86 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 1 | 6.72 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 10 | 6.71 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 14 | 6.69 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 3 | 6.57 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 12 | 6.47 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 7 | 6.34 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 11 | 6.21 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 9 | 6.17 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 16 | 6.13 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 4 | 6.05 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 19 | 5.82 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 2 | 5.74 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 6 | 5.74 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 9 | 5.63 |
| (1,43) | 1:34:A:ARG:C | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 14 | 5.51 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 14 | 5.39 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 19 | 5.27 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 9 | 5.2 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 17 | 5.17 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 15 | 5.06 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 2 | 4.95 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 16 | 4.94 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 17 | 4.83 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 6 | 4.74 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 16 | 4.7 |
| (1,18) | 1:18:A:GLY:N | 1:18:A:GLY:CA | 1:18:A:GLY:C | 1:19:A:ASN:N | 20 | 4.46 |
| (1,42) | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 1:34:A:ARG:N | 11 | 4.44 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 4 | 4.44 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1 | 4.44 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 6 | 4.43 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 14 | 4.41 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 2 | 4.36 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 14 | 4.32 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 3 | 4.28 |
| (1,9) | 1:5:A:ASN:C | 1:6:A:LEU:N | 1:6:A:LEU:CA | 1:6:A:LEU:C | 16 | 4.25 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 20 | 4.24 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 9 | 4.23 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 1 | 4.22 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 4 | 4.2 |
| (1,18) | 1:18:A:GLY:N | 1:18:A:GLY:CA | 1:18:A:GLY:C | 1:19:A:ASN:N | 16 | 4.1 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 8 | 4.08 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 9 | 4.07 |
| (1,50) | 1:40:A:ARG:N | 1:40:A:ARG:CA | 1:40:A:ARG:C | 1:41:A:CYS:N | 20 | 4.05 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 2 | 3.99 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 6 | 3.91 |
| (1,9) | 1:5:A:ASN:C | 1:6:A:LEU:N | 1:6:A:LEU:CA | 1:6:A:LEU:C | 18 | 3.89 |
| (1,2) | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 1:3:A:CYS:N | 15 | 3.87 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 9 | 3.86 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 13 | 3.78 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 10 | 3.69 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 5 | 3.67 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 17 | 3.66 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 20 | 3.63 |
| (1,18) | 1:18:A:GLY:N | 1:18:A:GLY:CA | 1:18:A:GLY:C | 1:19:A:ASN:N | 5 | 3.6 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 8 | 3.57 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 3 | 3.57 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 14 | 3.54 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 12 | 3.53 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 20 | 3.51 |
| (1,24) | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C | 1:24:A:CYS:N | 14 | 3.51 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 17 | 3.48 |
| (1,46) | 1:36:A:ARG:N | 1:36:A:ARG:CA | 1:36:A:ARG:C | 1:37:A:ASP:N | 3 | 3.46 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 9 | 3.46 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 13 | 3.43 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 4 | 3.34 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 8 | 3.27 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 18 | 3.25 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 19 | 3.22 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 11 | 3.2 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 16 | 3.18 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 6 | 3.09 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 20 | 3.06 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 16 | 3.04 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 5 | 3.02 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 20 | 3.02 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 15 | 3.01 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 18 | 2.99 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 6 | 2.99 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 14 | 2.94 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 1 | 2.91 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 4 | 2.91 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 15 | 2.91 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 12 | 2.83 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 7 | 2.81 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 13 | 2.81 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 18 | 2.81 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 15 | 2.78 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 14 | 2.76 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 11 | 2.72 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 14 | 2.71 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 18 | 2.7 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 7 | 2.63 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 12 | 2.61 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 8 | 2.59 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 1 | 2.56 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 19 | 2.56 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 3 | 2.55 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 12 | 2.51 |
| (1,9) | 1:5:A:ASN:C | 1:6:A:LEU:N | 1:6:A:LEU:CA | 1:6:A:LEU:C | 12 | 2.47 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 10 | 2.42 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 2 | 2.42 |
| (1,42) | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 1:34:A:ARG:N | 15 | 2.41 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 1 | 2.41 |
| (1,33) | 1:27:A:ASN:C | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 11 | 2.41 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 14 | 2.39 |
| (1,12) | 1:7:A:SER:N | 1:7:A:SER:CA | 1:7:A:SER:C | 1:8:A:GLY:N | 19 | 2.38 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 17 | 2.36 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 2 | 2.34 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 20 | 2.32 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 19 | 2.29 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 11 | 2.25 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 5 | 2.23 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 18 | 2.23 |
| (1,14) | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 1:11:A:LYS:N | 19 | 2.22 |
| (1,24) | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C | 1:24:A:CYS:N | 9 | 2.21 |
| (1,27) | 1:24:A:CYS:C | 1:25:A:ARG:N | 1:25:A:ARG:CA | 1:25:A:ARG:C | 9 | 2.18 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 20 | 2.13 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 11 | 2.13 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 13 | 2.12 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 16 | 2.12 |
| (1,18) | 1:18:A:GLY:N | 1:18:A:GLY:CA | 1:18:A:GLY:C | 1:19:A:ASN:N | 14 | 2.08 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 7 | 2.06 |
| (1,44) | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 1:36:A:ARG:N | 8 | 2.05 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 6 | 2.04 |
| (1,41) | 1:32:A:SER:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 19 | 2.02 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 18 | 2.02 |
| (1,42) | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 1:34:A:ARG:N | 5 | 2.0 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 20 | 2.0 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 3 | 1.99 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 11 | 1.96 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 6 | 1.93 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 11 | 1.93 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 6 | 1.93 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 12 | 1.91 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 15 | 1.89 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 16 | 1.87 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 5 | 1.84 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 20 | 1.83 |
| (1,24) | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C | 1:24:A:CYS:N | 1 | 1.83 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 3 | 1.82 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 13 | 1.8 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 14 | 1.8 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 17 | 1.73 |
| (1,27) | 1:24:A:CYS:C | 1:25:A:ARG:N | 1:25:A:ARG:CA | 1:25:A:ARG:C | 17 | 1.73 |
| (1,47) | 1:38:A:ASP:C | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 7 | 1.72 |
| (1,31) | 1:26:A:ASN:C | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 9 | 1.72 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 15 | 1.71 |
| (1,40) | 1:32:A:SER:N | 1:32:A:SER:CA | 1:32:A:SER:C | 1:33:A:GLY:N | 11 | 1.63 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 3 | 1.62 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 5 | 1.61 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 5 | 1.61 |
| (1,31) | 1:26:A:ASN:C | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 20 | 1.6 |
| (1,27) | 1:24:A:CYS:C | 1:25:A:ARG:N | 1:25:A:ARG:CA | 1:25:A:ARG:C | 4 | 1.58 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 12 | 1.58 |
| (1,9) | 1:5:A:ASN:C | 1:6:A:LEU:N | 1:6:A:LEU:CA | 1:6:A:LEU:C | 9 | 1.57 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 3 | 1.56 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 9 | 1.55 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 12 | 1.54 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 16 | 1.54 |
| (1,47) | 1:38:A:ASP:C | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 9 | 1.52 |
| (1,44) | 1:35:A:CYS:N | 1:35:A:CYS:CA | 1:35:A:CYS:C | 1:36:A:ARG:N | 10 | 1.51 |
| (1,27) | 1:24:A:CYS:C | 1:25:A:ARG:N | 1:25:A:ARG:CA | 1:25:A:ARG:C | 1 | 1.51 |
| (1,52) | 1:41:A:CYS:N | 1:41:A:CYS:CA | 1:41:A:CYS:C | 1:42:A:TRP:N | 6 | 1.5 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 6 | 1.5 |
| (1,41) | 1:32:A:SER:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 7 | 1.48 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 17 | 1.47 |
| (1,58) | 1:46:A:ARG:N | 1:46:A:ARG:CA | 1:46:A:ARG:C | 1:47:A:CYS:N | 20 | 1.44 |
| (1,42) | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 1:34:A:ARG:N | 2 | 1.44 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 18 | 1.44 |
| (1,42) | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 1:34:A:ARG:N | 6 | 1.43 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 4 | 1.43 |
| (1,41) | 1:32:A:SER:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 2 | 1.41 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 1 | 1.41 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 12 | 1.41 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 16 | 1.39 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 19 | 1.38 |
| (1,27) | 1:24:A:CYS:C | 1:25:A:ARG:N | 1:25:A:ARG:CA | 1:25:A:ARG:C | 19 | 1.38 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 10 | 1.37 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 17 | 1.35 |
| (1,31) | 1:26:A:ASN:C | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 3 | 1.33 |
| (1,31) | 1:26:A:ASN:C | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 4 | 1.31 |
| (1,32) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:GLU:N | 7 | 1.3 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,18) | 1:18:A:GLY:N | 1:18:A:GLY:CA | 1:18:A:GLY:C | 1:19:A:ASN:N | 1 | 1.29 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 4 | 1.28 |
| (1,13) | 1:9:A:THR:C | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 13 | 1.27 |
| (1,48) | 1:39:A:PHE:N | 1:39:A:PHE:CA | 1:39:A:PHE:C | 1:40:A:ARG:N | 12 | 1.26 |
| (1,38) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:SER:N | 7 | 1.26 |
| (1,27) | 1:24:A:CYS:C | 1:25:A:ARG:N | 1:25:A:ARG:CA | 1:25:A:ARG:C | 7 | 1.26 |
| (1,11) | 1:6:A:LEU:C | 1:7:A:SER:N | 1:7:A:SER:CA | 1:7:A:SER:C | 19 | 1.25 |
| (1,24) | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C | 1:24:A:CYS:N | 19 | 1.24 |
| (1,31) | 1:26:A:ASN:C | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 14 | 1.23 |
| (1,11) | 1:6:A:LEU:C | 1:7:A:SER:N | 1:7:A:SER:CA | 1:7:A:SER:C | 7 | 1.22 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 14 | 1.22 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 8 | 1.21 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 4 | 1.21 |
| (1,33) | 1:27:A:ASN:C | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 7 | 1.19 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 9 | 1.18 |
| (1,42) | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 1:34:A:ARG:N | 18 | 1.16 |
| (1,32) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:GLU:N | 6 | 1.15 |
| (1,58) | 1:46:A:ARG:N | 1:46:A:ARG:CA | 1:46:A:ARG:C | 1:47:A:CYS:N | 1 | 1.14 |
| (1,24) | 1:23:A:HIS:N | 1:23:A:HIS:CA | 1:23:A:HIS:C | 1:24:A:CYS:N | 4 | 1.14 |
| (1,9) | 1:5:A:ASN:C | 1:6:A:LEU:N | 1:6:A:LEU:CA | 1:6:A:LEU:C | 3 | 1.14 |
| (1,4) | 1:3:A:CYS:N | 1:3:A:CYS:CA | 1:3:A:CYS:C | 1:4:A:GLU:N | 11 | 1.14 |
| (1,31) | 1:26:A:ASN:C | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 6 | 1.13 |
| (1,37) | 1:30:A:LEU:C | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 7 | 1.12 |
| (1,18) | 1:18:A:GLY:N | 1:18:A:GLY:CA | 1:18:A:GLY:C | 1:19:A:ASN:N | 10 | 1.1 |
| (1,14) | 1:10:A:PHE:N | 1:10:A:PHE:CA | 1:10:A:PHE:C | 1:11:A:LYS:N | 3 | 1.09 |
| (1,33) | 1:27:A:ASN:C | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 19 | 1.08 |
| (1,34) | 1:28:A:GLU:N | 1:28:A:GLU:CA | 1:28:A:GLU:C | 1:29:A:HIS:N | 19 | 1.04 |
| (1,32) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:GLU:N | 12 | 1.04 |
| (1,16) | 1:17:A:ASP:N | 1:17:A:ASP:CA | 1:17:A:ASP:C | 1:18:A:GLY:N | 19 | 1.02 |
| (1,1) | 1:1:A:LYS:C | 1:2:A:THR:N | 1:2:A:THR:CA | 1:2:A:THR:C | 2 | 1.0 |