



Full wwPDB NMR Structure Validation Report i

Dec 13, 2023 – 06:20 PM EST

PDB ID : 2JOZ
BMRB ID : 15211
Title : Solution NMR structure of protein yxeF, Northeast Structural Genomics Consortium target Sr500a
Authors : Wu, Y.; Liu, G.; Zhang, Q.; Bhatnagar, S.; Chen, C.; Nwosu, C.; Xiao, R.; Cunningham, K.; Locke, J.; Ma, L.; Swapna, G.; Baran, M.; Acton, T.; Montelione, G.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2007-04-10

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 i 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 \(1\)](#)) were used in the production of this report:

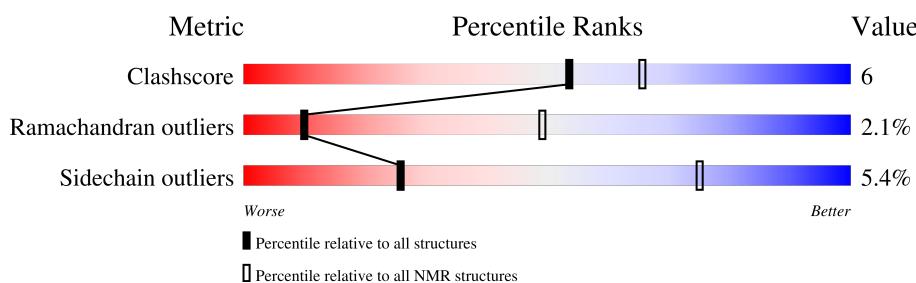
| | | |
|--------------------------------|---|--|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbit | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| BMRB Restraints Analysis | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

1 Overall quality at a glance [\(i\)](#)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 135 | 69% .. 26% |

2 Ensemble composition and analysis i

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:14-A:113 (100) | 1.18 | 17 |

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition [\(i\)](#)

There is only 1 type of molecule in this entry. The entry contains 2126 atoms, of which 1043 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein yxeF.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| | | | Total | C | H | N | O | S | |
| 1 | A | 135 | 2126 | 672 | 1043 | 187 | 218 | 6 | 0 |

There are 9 discrepancies between the modelled and reference sequences:

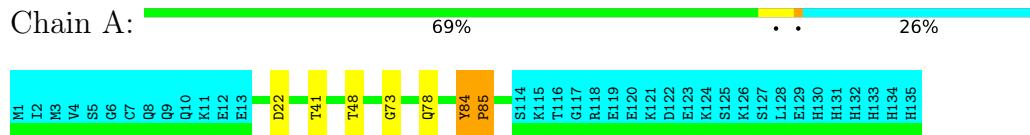
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| A | 1 | MET | - | initiating methionine | UNP P54945 |
| A | 128 | LEU | - | cloning artifact | UNP P54945 |
| A | 129 | GLU | - | cloning artifact | UNP P54945 |
| A | 130 | HIS | - | expression tag | UNP P54945 |
| A | 131 | HIS | - | expression tag | UNP P54945 |
| A | 132 | HIS | - | expression tag | UNP P54945 |
| A | 133 | HIS | - | expression tag | UNP P54945 |
| A | 134 | HIS | - | expression tag | UNP P54945 |
| A | 135 | HIS | - | expression tag | UNP P54945 |

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: Hypothetical protein yxeF

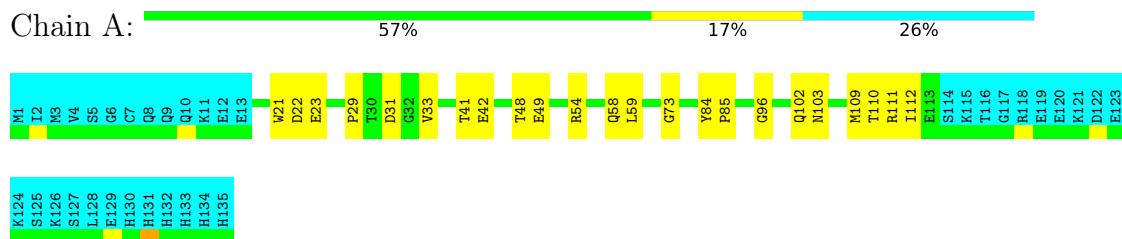


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

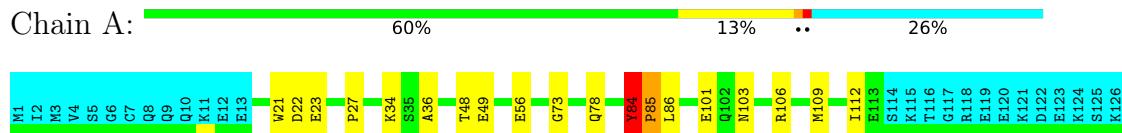
4.2.1 Score per residue for model 1

- Molecule 1: Hypothetical protein yxeF



4.2.2 Score per residue for model 2

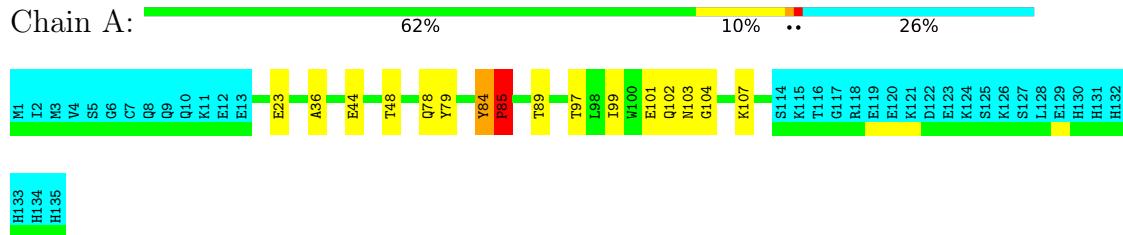
- Molecule 1: Hypothetical protein yxeF





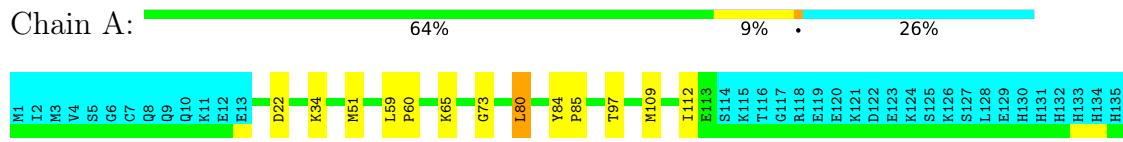
4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical protein yxeF



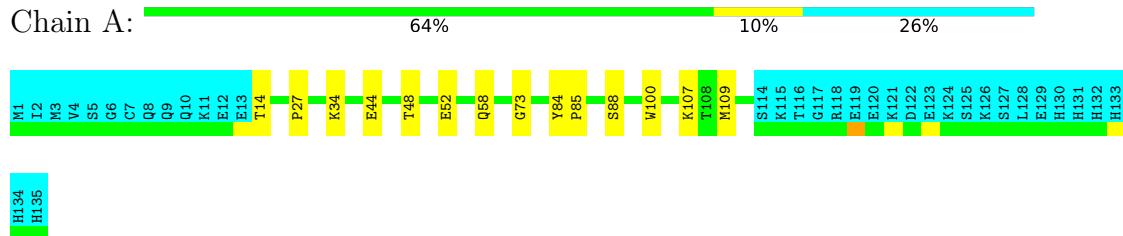
4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein yxeF



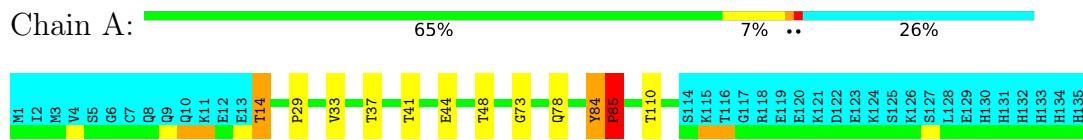
4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical protein yxeF



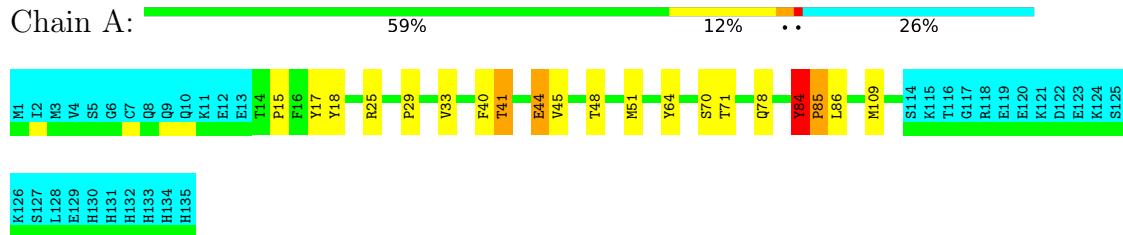
4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein yxeF



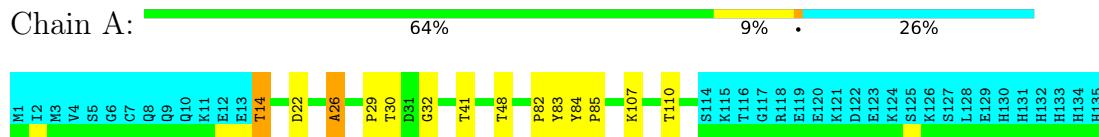
4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein yxeF



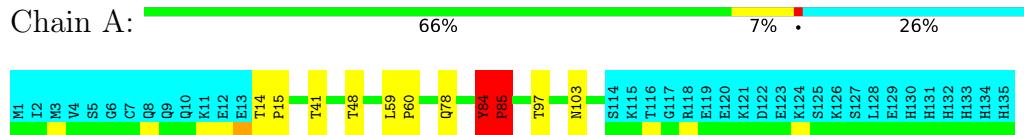
4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein yxeF



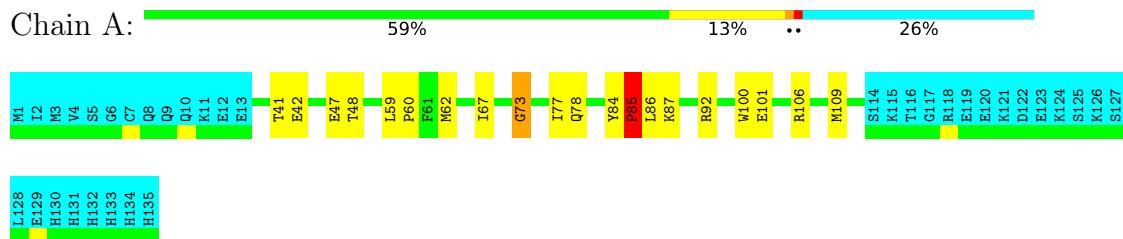
4.2.9 Score per residue for model 9

- Molecule 1: Hypothetical protein yxeF



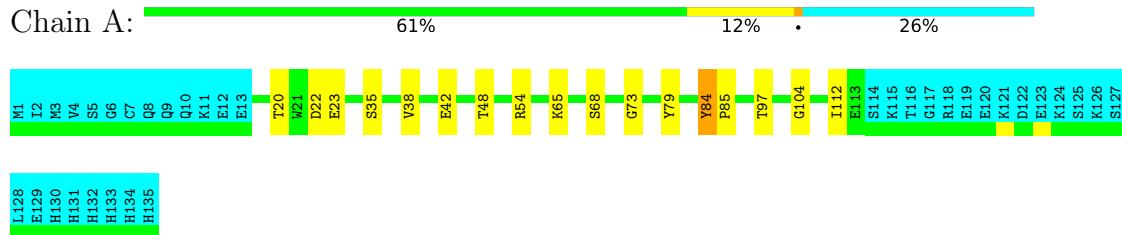
4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein yxeF



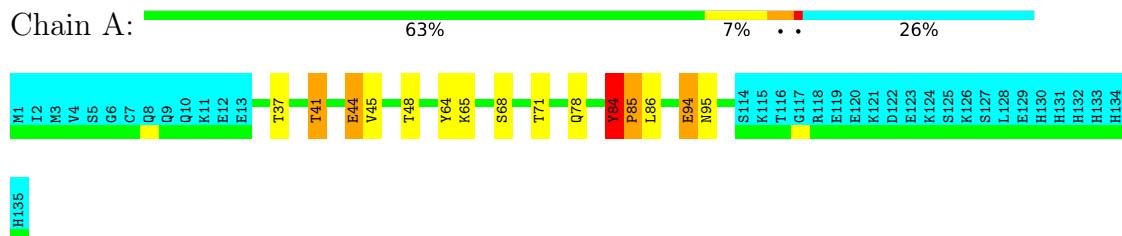
4.2.11 Score per residue for model 11

- Molecule 1: Hypothetical protein yxeF



4.2.12 Score per residue for model 12

- Molecule 1: Hypothetical protein yxeF



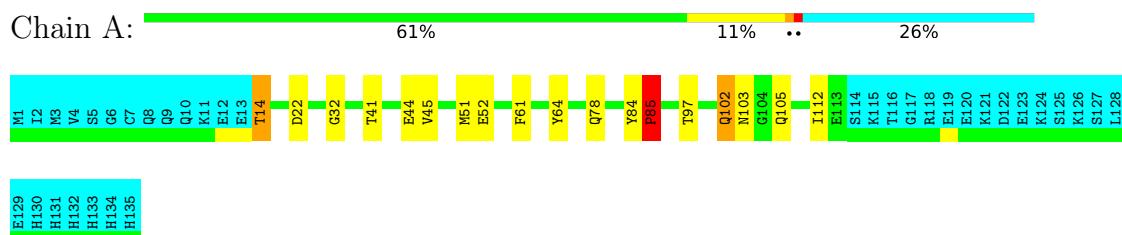
4.2.13 Score per residue for model 13

- Molecule 1: Hypothetical protein yxeF



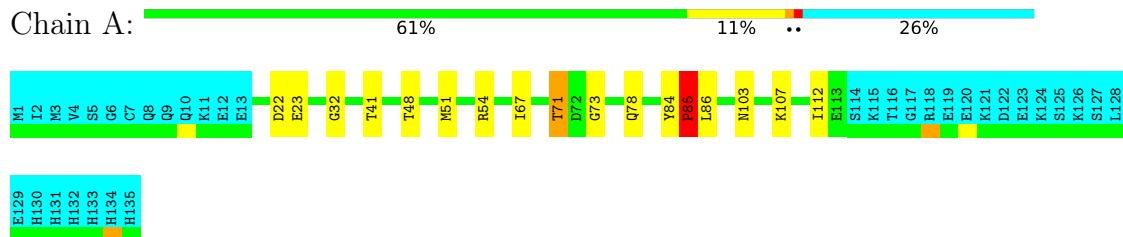
4.2.14 Score per residue for model 14

- Molecule 1: Hypothetical protein yxeF



4.2.15 Score per residue for model 15

- Molecule 1: Hypothetical protein yxeF



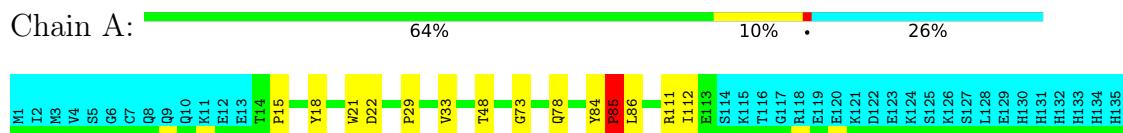
4.2.16 Score per residue for model 16

- Molecule 1: Hypothetical protein yxeF



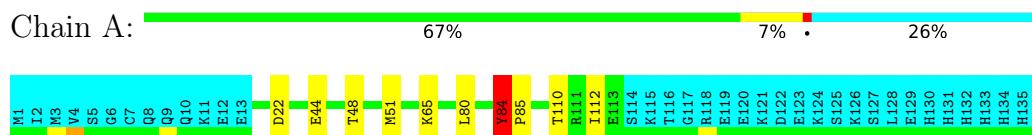
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Hypothetical protein yxeF



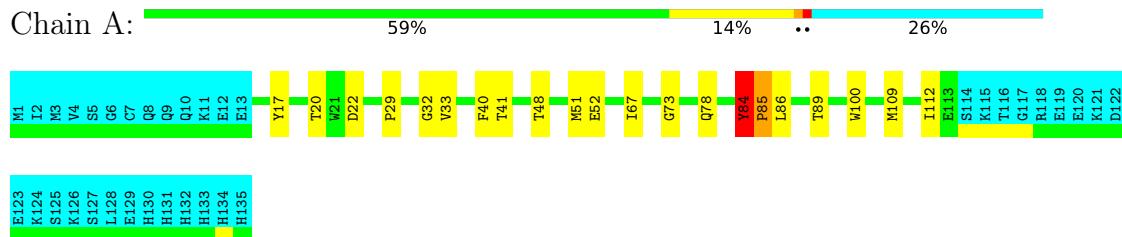
4.2.18 Score per residue for model 18

- Molecule 1: Hypothetical protein yxeF



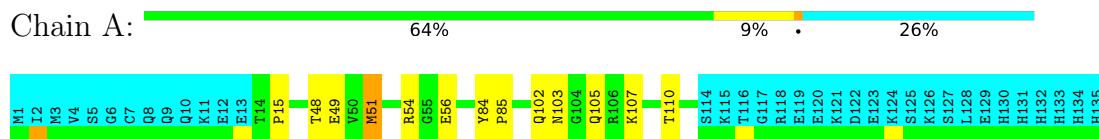
4.2.19 Score per residue for model 19

- Molecule 1: Hypothetical protein yxeF



4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical protein yxeF



5 Refinement protocol and experimental data overview i

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

Of the 100 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 |
|---------------|--------------------|---------|
| CYANA | structure solution | 2.1 |
| AutoStructure | structure solution | 1.0 |
| CNS | refinement | 1.1 |

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

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1559 |
| Number of shifts mapped to atoms | 1559 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 91% |

6 Model quality i

6.1 Standard geometry i

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------------|-------------|-----------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.36±0.01 | 0±0/812 (0.0± 0.0%) | 0.47±0.03 | 0±0/1103 (0.0± 0.0%) |
| All | All | 0.36 | 0/16240 (0.0%) | 0.47 | 9/22060 (0.0%) |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 0.0±0.0 | 0.4±0.5 |
| All | All | 0 | 8 |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 85 | PRO | CA-N-CD | -5.48 | 103.83 | 111.50 | 6 | 9 |

There are no chirality outliers.

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|---------|----------------|
| 1 | A | 84 | TYR | Peptide | 8 |

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 | 793 | 764 | 764 | 9±3 |
| All | All | 15860 | 15280 | 15280 | 172 |

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 6.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:84:TYR:HB2 | 1:A:85:PRO:HD2 | 0.82 | 1.47 | 16 | 12 |
| 1:A:78:GLN:NE2 | 1:A:85:PRO:HA | 0.78 | 1.93 | 7 | 10 |
| 1:A:34:LYS:HE2 | 1:A:34:LYS:HA | 0.71 | 1.63 | 13 | 2 |
| 1:A:23:GLU:O | 1:A:23:GLU:HG3 | 0.66 | 1.91 | 1 | 1 |
| 1:A:14:THR:HB | 1:A:15:PRO:HD3 | 0.66 | 1.66 | 9 | 1 |
| 1:A:84:TYR:HB2 | 1:A:85:PRO:CD | 0.63 | 2.23 | 7 | 9 |
| 1:A:34:LYS:HE3 | 1:A:52:GLU:HB3 | 0.63 | 1.71 | 16 | 1 |
| 1:A:86:LEU:HG | 1:A:102:GLN:HE22 | 0.63 | 1.53 | 16 | 1 |
| 1:A:100:TRP:HB2 | 1:A:109:MET:SD | 0.62 | 2.33 | 10 | 1 |
| 1:A:35:SER:HB2 | 1:A:50:VAL:HB | 0.60 | 1.73 | 16 | 1 |
| 1:A:79:TYR:O | 1:A:84:TYR:HA | 0.59 | 1.97 | 11 | 2 |
| 1:A:84:TYR:CB | 1:A:85:PRO:HD2 | 0.59 | 2.26 | 9 | 12 |
| 1:A:29:PRO:HG2 | 1:A:33:VAL:HB | 0.58 | 1.73 | 16 | 1 |
| 1:A:22:ASP:HB2 | 1:A:112:ILE:HD11 | 0.56 | 1.78 | 1 | 8 |
| 1:A:33:VAL:HG11 | 1:A:49:GLU:HB3 | 0.56 | 1.77 | 1 | 1 |
| 1:A:29:PRO:HD2 | 1:A:33:VAL:HB | 0.53 | 1.80 | 17 | 2 |
| 1:A:84:TYR:N | 1:A:85:PRO:CD | 0.53 | 2.72 | 18 | 7 |
| 1:A:34:LYS:HE3 | 1:A:52:GLU:HB2 | 0.52 | 1.81 | 5 | 1 |
| 1:A:100:TRP:HE3 | 1:A:109:MET:HE1 | 0.52 | 1.64 | 5 | 1 |
| 1:A:78:GLN:CD | 1:A:85:PRO:HA | 0.52 | 2.24 | 3 | 4 |
| 1:A:25:ARG:HH11 | 1:A:26:ALA:HB2 | 0.51 | 1.66 | 13 | 1 |
| 1:A:15:PRO:HB2 | 1:A:18:TYR:HB2 | 0.50 | 1.82 | 7 | 2 |
| 1:A:49:GLU:O | 1:A:56:GLU:HA | 0.50 | 2.06 | 20 | 2 |
| 1:A:62:MET:CE | 1:A:62:MET:HA | 0.49 | 2.37 | 10 | 1 |
| 1:A:84:TYR:CD2 | 1:A:85:PRO:HD2 | 0.49 | 2.42 | 6 | 3 |
| 1:A:65:LYS:HG3 | 1:A:80:LEU:HD11 | 0.48 | 1.83 | 4 | 1 |
| 1:A:73:GLY:HA3 | 1:A:92:ARG:HH11 | 0.48 | 1.68 | 10 | 1 |
| 1:A:84:TYR:CG | 1:A:85:PRO:CD | 0.48 | 2.96 | 19 | 1 |
| 1:A:86:LEU:HD13 | 1:A:87:LYS:N | 0.47 | 2.24 | 10 | 1 |
| 1:A:107:LYS:HE2 | 1:A:107:LYS:HA | 0.47 | 1.86 | 5 | 3 |
| 1:A:22:ASP:CB | 1:A:112:ILE:HD11 | 0.47 | 2.40 | 15 | 2 |
| 1:A:84:TYR:CD1 | 1:A:85:PRO:HD3 | 0.47 | 2.44 | 1 | 2 |
| 1:A:102:GLN:OE1 | 1:A:103:ASN:HB2 | 0.46 | 2.09 | 3 | 1 |
| 1:A:77:ILE:O | 1:A:87:LYS:HB2 | 0.46 | 2.11 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:84:TYR:O | 1:A:86:LEU:N | 0.46 | 2.48 | 19 | 9 |
| 1:A:21:TRP:CZ3 | 1:A:111:ARG:HB2 | 0.46 | 2.44 | 17 | 2 |
| 1:A:101:GLU:HG2 | 1:A:106:ARG:HB3 | 0.46 | 1.87 | 13 | 2 |
| 1:A:23:GLU:HB2 | 1:A:35:SER:HB3 | 0.46 | 1.86 | 11 | 1 |
| 1:A:45:VAL:HG23 | 1:A:64:TYR:CD1 | 0.45 | 2.45 | 12 | 3 |
| 1:A:67:ILE:HD11 | 1:A:78:GLN:HB2 | 0.45 | 1.88 | 15 | 4 |
| 1:A:41:THR:HG22 | 1:A:42:GLU:H | 0.45 | 1.71 | 10 | 2 |
| 1:A:41:THR:HB | 1:A:44:GLU:HB2 | 0.45 | 1.88 | 6 | 1 |
| 1:A:17:TYR:O | 1:A:40:PHE:HB2 | 0.45 | 2.12 | 7 | 2 |
| 1:A:101:GLU:HG2 | 1:A:106:ARG:HG2 | 0.45 | 1.87 | 10 | 1 |
| 1:A:84:TYR:C | 1:A:86:LEU:H | 0.45 | 2.15 | 12 | 4 |
| 1:A:26:ALA:HB3 | 1:A:107:LYS:HE2 | 0.45 | 1.87 | 8 | 1 |
| 1:A:29:PRO:O | 1:A:30:THR:HB | 0.44 | 2.13 | 8 | 1 |
| 1:A:20:THR:HA | 1:A:38:VAL:O | 0.44 | 2.11 | 11 | 1 |
| 1:A:51:MET:HB3 | 1:A:54:ARG:HG2 | 0.44 | 1.90 | 20 | 1 |
| 1:A:21:TRP:HB3 | 1:A:109:MET:HB3 | 0.44 | 1.89 | 1 | 2 |
| 1:A:41:THR:HB | 1:A:44:GLU:OE2 | 0.44 | 2.13 | 12 | 2 |
| 1:A:29:PRO:HG2 | 1:A:33:VAL:HG21 | 0.43 | 1.91 | 6 | 1 |
| 1:A:84:TYR:CB | 1:A:85:PRO:CD | 0.43 | 2.96 | 9 | 3 |
| 1:A:59:LEU:HB3 | 1:A:60:PRO:HD2 | 0.43 | 1.89 | 4 | 3 |
| 1:A:29:PRO:HD2 | 1:A:33:VAL:HG21 | 0.43 | 1.88 | 13 | 1 |
| 1:A:78:GLN:HE21 | 1:A:85:PRO:HA | 0.43 | 1.74 | 19 | 1 |
| 1:A:22:ASP:HB2 | 1:A:112:ILE:HG12 | 0.42 | 1.90 | 2 | 1 |
| 1:A:84:TYR:CG | 1:A:85:PRO:HD2 | 0.42 | 2.49 | 12 | 1 |
| 1:A:37:THR:OG1 | 1:A:48:THR:HB | 0.42 | 2.14 | 12 | 1 |
| 1:A:23:GLU:CD | 1:A:107:LYS:HD3 | 0.42 | 2.35 | 15 | 1 |
| 1:A:100:TRP:HB2 | 1:A:109:MET:CE | 0.42 | 2.45 | 19 | 1 |
| 1:A:99:ILE:HA | 1:A:107:LYS:O | 0.42 | 2.14 | 3 | 1 |
| 1:A:27:PRO:HA | 1:A:34:LYS:O | 0.42 | 2.15 | 2 | 1 |
| 1:A:47:GLU:HB2 | 1:A:59:LEU:HB2 | 0.42 | 1.92 | 10 | 1 |
| 1:A:34:LYS:CE | 1:A:52:GLU:HB3 | 0.42 | 2.42 | 16 | 1 |
| 1:A:22:ASP:HB3 | 1:A:112:ILE:HD11 | 0.41 | 1.91 | 15 | 1 |
| 1:A:102:GLN:O | 1:A:105:GLN:HG2 | 0.41 | 2.15 | 14 | 2 |
| 1:A:89:THR:HB | 1:A:101:GLU:HB2 | 0.41 | 1.92 | 3 | 1 |
| 1:A:82:PRO:HG2 | 1:A:83:TYR:CE2 | 0.41 | 2.50 | 8 | 1 |
| 1:A:51:MET:SD | 1:A:54:ARG:HG3 | 0.41 | 2.56 | 15 | 1 |
| 1:A:29:PRO:HG2 | 1:A:33:VAL:CG2 | 0.41 | 2.45 | 6 | 1 |
| 1:A:33:VAL:HG22 | 1:A:51:MET:HG2 | 0.41 | 1.91 | 19 | 1 |
| 1:A:94:GLU:HG2 | 1:A:95:ASN:ND2 | 0.40 | 2.31 | 12 | 1 |
| 1:A:44:GLU:HB2 | 1:A:61:PHE:HB2 | 0.40 | 1.93 | 14 | 1 |
| 1:A:54:ARG:HG3 | 1:A:55:GLY:N | 0.40 | 2.31 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:23:GLU:HG3 | 1:A:36:ALA:O | 0.40 | 2.16 | 2 | 1 |
| 1:A:23:GLU:HG2 | 1:A:36:ALA:O | 0.40 | 2.17 | 3 | 1 |
| 1:A:94:GLU:H | 1:A:94:GLU:CD | 0.40 | 2.19 | 12 | 1 |
| 1:A:65:LYS:HG2 | 1:A:80:LEU:HD11 | 0.40 | 1.93 | 18 | 1 |

6.3 Torsion angles [\(i\)](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|--------------|------------|------------|-------------|
| 1 | A | 100/135 (74%) | 91±1 (91±1%) | 7±2 (7±2%) | 2±1 (2±1%) | 10 49 |
| All | All | 2000/2700 (74%) | 1811 (91%) | 146 (7%) | 43 (2%) | 10 49 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 85 | PRO | 13 |
| 1 | A | 73 | GLY | 10 |
| 1 | A | 32 | GLY | 5 |
| 1 | A | 14 | THR | 4 |
| 1 | A | 29 | PRO | 2 |
| 1 | A | 104 | GLY | 2 |
| 1 | A | 26 | ALA | 2 |
| 1 | A | 84 | TYR | 2 |
| 1 | A | 96 | GLY | 1 |
| 1 | A | 80 | LEU | 1 |
| 1 | A | 27 | PRO | 1 |

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|--------------|------------|-------------|
| 1 | A | 86/119 (72%) | 81±2 (95±2%) | 5±2 (5±2%) | 26 75 |
| All | All | 1720/2380 (72%) | 1627 (95%) | 93 (5%) | 26 75 |

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 | 48 | THR | 17 |
| 1 | A | 41 | THR | 8 |
| 1 | A | 103 | ASN | 7 |
| 1 | A | 110 | THR | 7 |
| 1 | A | 84 | TYR | 7 |
| 1 | A | 85 | PRO | 7 |
| 1 | A | 97 | THR | 6 |
| 1 | A | 44 | GLU | 5 |
| 1 | A | 51 | MET | 5 |
| 1 | A | 71 | THR | 4 |
| 1 | A | 54 | ARG | 2 |
| 1 | A | 102 | GLN | 2 |
| 1 | A | 109 | MET | 2 |
| 1 | A | 88 | SER | 2 |
| 1 | A | 65 | LYS | 2 |
| 1 | A | 68 | SER | 2 |
| 1 | A | 52 | GLU | 2 |
| 1 | A | 37 | THR | 1 |
| 1 | A | 25 | ARG | 1 |
| 1 | A | 22 | ASP | 1 |
| 1 | A | 42 | GLU | 1 |
| 1 | A | 94 | GLU | 1 |
| 1 | A | 89 | THR | 1 |

6.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

| | |
|---|------|
| Total number of shifts | 1559 |
| Number of shifts mapped to atoms | 1559 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 5 |

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|-------------------------|
| $^{13}\text{C}_\alpha$ | 128 | -0.23 \pm 0.09 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 115 | 0.02 \pm 0.10 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 121 | -0.13 \pm 0.14 | None needed (< 0.5 ppm) |
| ^{15}N | 122 | -0.45 \pm 0.35 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1220 atoms were assigned a chemical shift out of a possible 1335. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 493/499 (99%) | 205/205 (100%) | 194/200 (97%) | 94/94 (100%) |
| Sidechain | 644/728 (88%) | 436/470 (93%) | 201/231 (87%) | 7/27 (26%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 83/108 (77%) | 51/51 (100%) | 30/55 (55%) | 2/2 (100%) |
| Overall | 1220/1335 (91%) | 692/726 (95%) | 425/486 (87%) | 103/123 (84%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1556 atoms were assigned a chemical shift out of a possible 1814. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 634/676 (94%) | 263/277 (95%) | 249/270 (92%) | 122/129 (95%) |
| Sidechain | 839/982 (85%) | 569/630 (90%) | 263/314 (84%) | 7/38 (18%) |
| Aromatic | 83/156 (53%) | 51/75 (68%) | 30/67 (45%) | 2/14 (14%) |
| Overall | 1556/1814 (86%) | 883/982 (90%) | 542/651 (83%) | 131/181 (72%) |

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

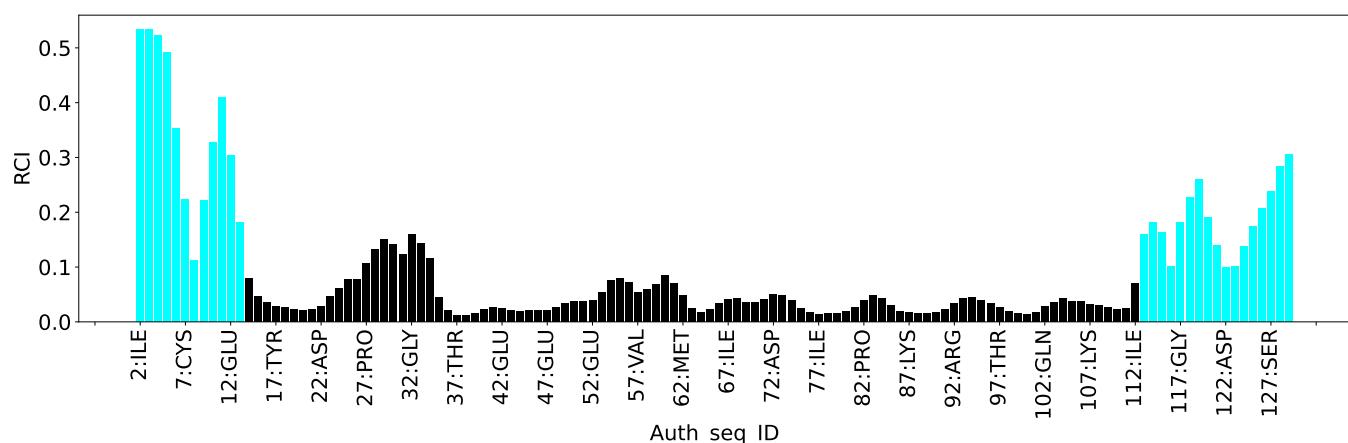
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 15 | PRO | HB2 | 0.03 | 0.37 – 3.78 | -6.0 |
| 1 | A | 98 | LEU | HB2 | -0.41 | -0.07 – 3.30 | -6.0 |
| 1 | A | 98 | LEU | HD21 | -0.67 | -0.65 – 2.13 | -5.1 |
| 1 | A | 98 | LEU | HD22 | -0.67 | -0.65 – 2.13 | -5.1 |
| 1 | A | 98 | LEU | HD23 | -0.67 | -0.65 – 2.13 | -5.1 |

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 i

8.1 Conformationally restricting restraints i

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 | 1666 |
| Intra-residue ($ i-j =0$) | 439 |
| Sequential ($ i-j =1$) | 507 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 132 |
| Long range ($ i-j \geq 5$) | 588 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 202 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 13.8 |
| Number of long range restraints per residue ¹ | 4.4 |

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 i

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 i

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) | 19.1 | 0.2 |
| 0.2-0.5 (Medium) | 16.1 | 0.5 |
| >0.5 (Large) | 10.7 | 2.65 |

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) | 15.6 | 9.86 |
| 10.0-20.0 (Medium) | 0.3 | 19.62 |
| >20.0 (Large) | 1.1 | 146.65 |

9 Distance violation analysis (i)

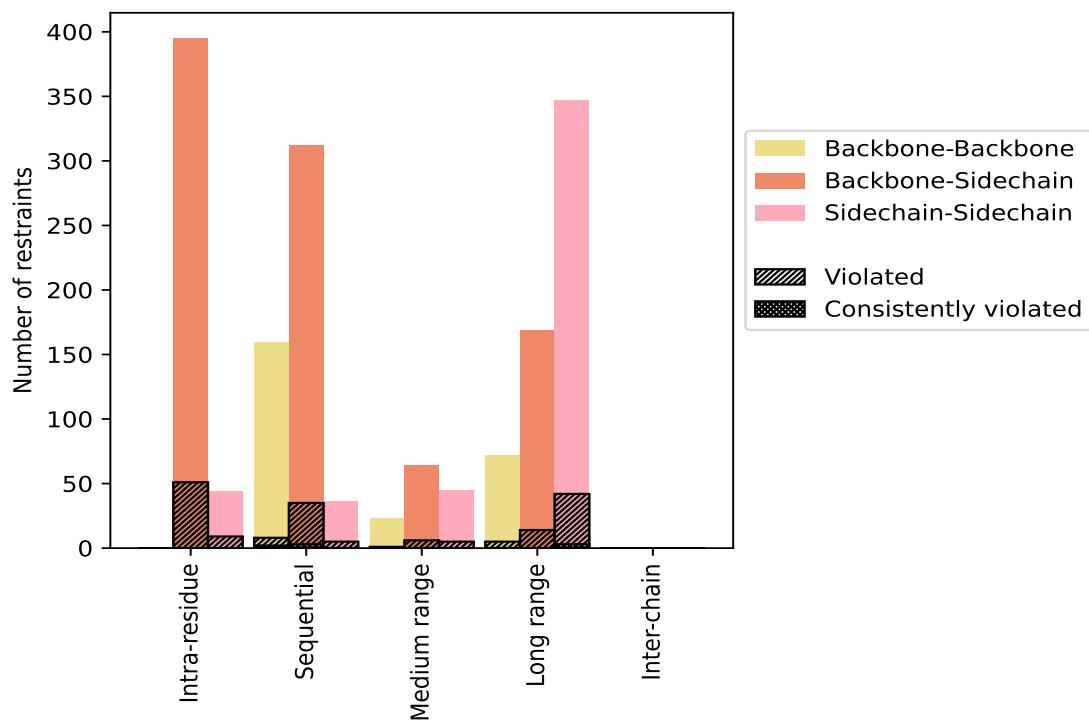
9.1 Summary of distance violations (i)

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

| Restraints type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($ i-j =0$) | 439 | 26.4 | 60 | 13.7 | 3.6 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 395 | 23.7 | 51 | 12.9 | 3.1 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 44 | 2.6 | 9 | 20.5 | 0.5 | 0 | 0.0 | 0.0 |
| Sequential ($ i-j =1$) | 507 | 30.4 | 48 | 9.5 | 2.9 | 5 | 1.0 | 0.3 |
| Backbone-Backbone | 159 | 9.5 | 8 | 5.0 | 0.5 | 2 | 1.3 | 0.1 |
| Backbone-Sidechain | 312 | 18.7 | 35 | 11.2 | 2.1 | 3 | 1.0 | 0.2 |
| Sidechain-Sidechain | 36 | 2.2 | 5 | 13.9 | 0.3 | 0 | 0.0 | 0.0 |
| Medium range ($ i-j >1 \text{ & } i-j <5$) | 132 | 7.9 | 12 | 9.1 | 0.7 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 23 | 1.4 | 1 | 4.3 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 64 | 3.8 | 6 | 9.4 | 0.4 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 45 | 2.7 | 5 | 11.1 | 0.3 | 0 | 0.0 | 0.0 |
| Long range ($ i-j \geq 5$) | 588 | 35.3 | 61 | 10.4 | 3.7 | 3 | 0.5 | 0.2 |
| Backbone-Backbone | 72 | 4.3 | 5 | 6.9 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 169 | 10.1 | 14 | 8.3 | 0.8 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 347 | 20.8 | 42 | 12.1 | 2.5 | 3 | 0.9 | 0.2 |
| 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 | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 1666 | 100.0 | 181 | 10.9 | 10.9 | 8 | 0.5 | 0.5 |
| Backbone-Backbone | 254 | 15.2 | 14 | 5.5 | 0.8 | 2 | 0.8 | 0.1 |
| Backbone-Sidechain | 940 | 56.4 | 106 | 11.3 | 6.4 | 3 | 0.3 | 0.2 |
| Sidechain-Sidechain | 472 | 28.3 | 61 | 12.9 | 3.7 | 3 | 0.6 | 0.2 |

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 | 17 | 14 | 3 | 21 | 0 | 55 | 0.43 | 1.81 | 0.44 | 0.24 |
| 2 | 10 | 13 | 5 | 12 | 0 | 40 | 0.46 | 2.15 | 0.5 | 0.23 |
| 3 | 11 | 14 | 3 | 11 | 0 | 39 | 0.45 | 1.59 | 0.43 | 0.23 |
| 4 | 14 | 9 | 5 | 12 | 0 | 40 | 0.42 | 2.12 | 0.49 | 0.24 |
| 5 | 11 | 13 | 3 | 16 | 0 | 43 | 0.39 | 1.81 | 0.41 | 0.2 |
| 6 | 15 | 15 | 2 | 16 | 0 | 48 | 0.4 | 1.95 | 0.4 | 0.24 |
| 7 | 9 | 12 | 5 | 22 | 0 | 48 | 0.41 | 2.65 | 0.5 | 0.22 |
| 8 | 17 | 17 | 5 | 16 | 0 | 55 | 0.45 | 1.89 | 0.48 | 0.2 |
| 9 | 18 | 13 | 3 | 19 | 0 | 53 | 0.39 | 2.04 | 0.39 | 0.21 |
| 10 | 18 | 19 | 2 | 24 | 0 | 63 | 0.4 | 2.08 | 0.43 | 0.21 |
| 11 | 10 | 13 | 4 | 17 | 0 | 44 | 0.43 | 1.8 | 0.46 | 0.21 |

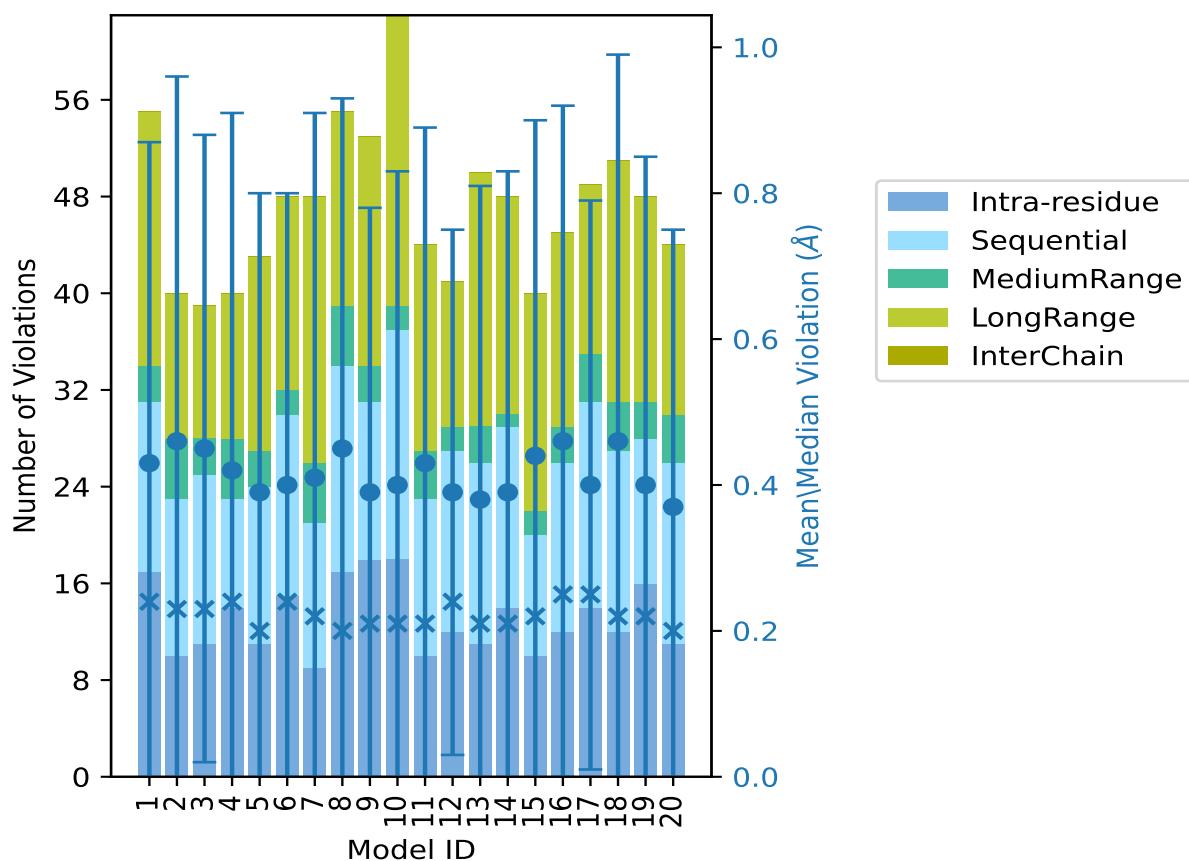
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 12 | 12 | 15 | 2 | 12 | 0 | 41 | 0.39 | 1.6 | 0.36 | 0.24 |
| 13 | 11 | 15 | 3 | 21 | 0 | 50 | 0.38 | 2.13 | 0.43 | 0.21 |
| 14 | 14 | 15 | 1 | 18 | 0 | 48 | 0.39 | 2.22 | 0.44 | 0.21 |
| 15 | 10 | 10 | 2 | 18 | 0 | 40 | 0.44 | 1.83 | 0.46 | 0.22 |
| 16 | 12 | 14 | 3 | 16 | 0 | 45 | 0.46 | 1.98 | 0.46 | 0.25 |
| 17 | 14 | 17 | 4 | 14 | 0 | 49 | 0.4 | 1.82 | 0.39 | 0.25 |
| 18 | 12 | 15 | 4 | 20 | 0 | 51 | 0.46 | 2.57 | 0.53 | 0.22 |
| 19 | 16 | 12 | 3 | 17 | 0 | 48 | 0.4 | 1.78 | 0.45 | 0.22 |
| 20 | 11 | 15 | 4 | 14 | 0 | 44 | 0.37 | 1.57 | 0.38 | 0.2 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,
⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

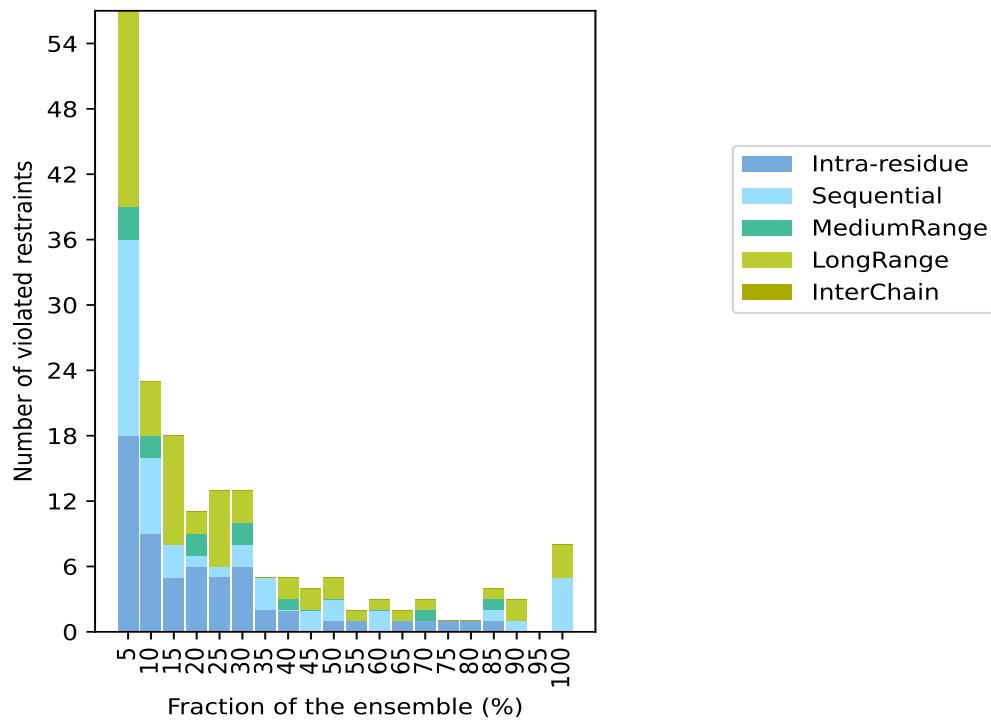
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1485(IR:379, SQ:459, MR:120, LR:527, IC:0) restraints are not violated in the ensemble.

| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Fraction of the ensemble | |
|-----------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| | | | | | | Count ⁶ | % |
| 18 | 18 | 3 | 18 | 0 | 57 | 1 | 5.0 |
| 9 | 7 | 2 | 5 | 0 | 23 | 2 | 10.0 |
| 5 | 3 | 0 | 10 | 0 | 18 | 3 | 15.0 |
| 6 | 1 | 2 | 2 | 0 | 11 | 4 | 20.0 |
| 5 | 1 | 0 | 7 | 0 | 13 | 5 | 25.0 |
| 6 | 2 | 2 | 3 | 0 | 13 | 6 | 30.0 |
| 2 | 3 | 0 | 0 | 0 | 5 | 7 | 35.0 |
| 2 | 0 | 1 | 2 | 0 | 5 | 8 | 40.0 |
| 0 | 2 | 0 | 2 | 0 | 4 | 9 | 45.0 |
| 1 | 2 | 0 | 2 | 0 | 5 | 10 | 50.0 |
| 1 | 0 | 0 | 1 | 0 | 2 | 11 | 55.0 |
| 0 | 2 | 0 | 1 | 0 | 3 | 12 | 60.0 |
| 1 | 0 | 0 | 1 | 0 | 2 | 13 | 65.0 |
| 1 | 0 | 1 | 1 | 0 | 3 | 14 | 70.0 |
| 1 | 0 | 0 | 0 | 0 | 1 | 15 | 75.0 |
| 1 | 0 | 0 | 0 | 0 | 1 | 16 | 80.0 |
| 1 | 1 | 1 | 1 | 0 | 4 | 17 | 85.0 |
| 0 | 1 | 0 | 2 | 0 | 3 | 18 | 90.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 19 | 95.0 |
| 0 | 5 | 0 | 3 | 0 | 8 | 20 | 100.0 |

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

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

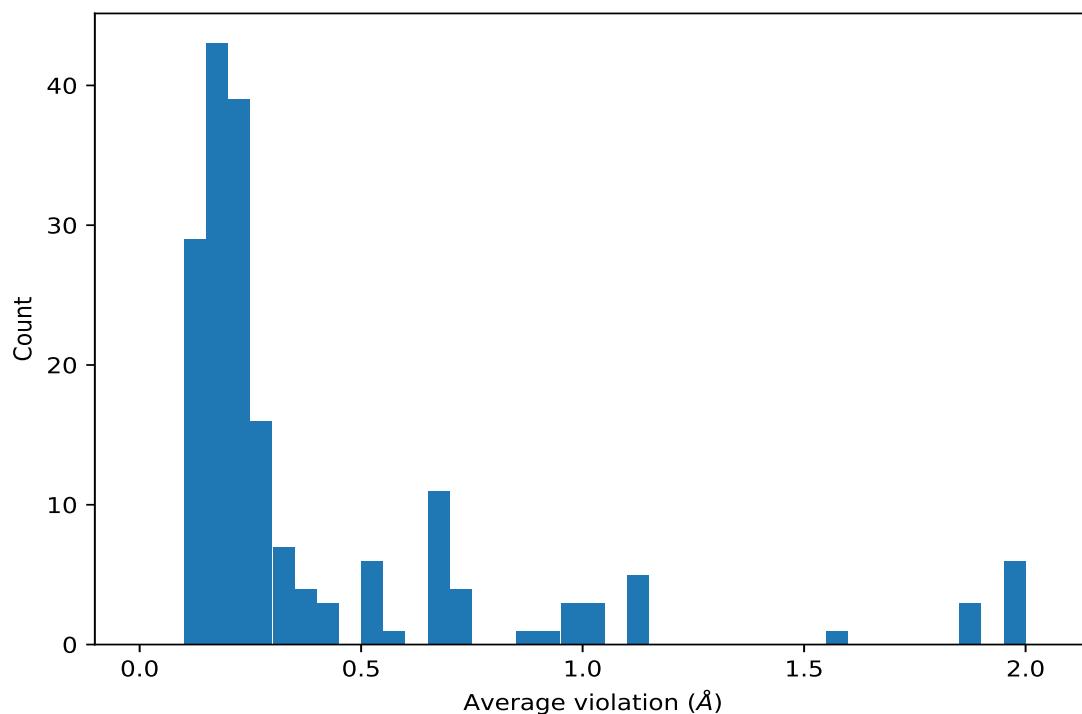
9.3.1 Bar graph : Distance violation statistics for the ensemble [\(i\)](#)



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) |
|----------|-----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 20 | 1.85 | 0.26 | 1.87 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 20 | 1.85 | 0.26 | 1.87 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 20 | 1.85 | 0.26 | 1.87 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 20 | 1.59 | 0.07 | 1.57 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 20 | 1.13 | 0.24 | 1.0 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 20 | 0.96 | 0.09 | 0.94 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 20 | 0.96 | 0.09 | 0.94 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 20 | 0.93 | 0.56 | 1.32 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 20 | 0.86 | 0.12 | 0.83 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 20 | 0.74 | 0.23 | 0.75 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 20 | 0.74 | 0.23 | 0.75 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 20 | 0.74 | 0.23 | 0.75 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 20 | 0.68 | 0.2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 20 | 0.68 | 0.2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 20 | 0.68 | 0.2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 20 | 0.68 | 0.2 | 0.71 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 20 | 0.68 | 0.2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 20 | 0.68 | 0.2 | 0.71 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 18 | 0.34 | 0.05 | 0.34 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 18 | 0.24 | 0.03 | 0.24 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 18 | 0.19 | 0.03 | 0.2 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 17 | 0.24 | 0.05 | 0.23 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 17 | 0.23 | 0.03 | 0.23 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 17 | 0.2 | 0.04 | 0.19 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 17 | 0.2 | 0.04 | 0.19 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 17 | 0.19 | 0.05 | 0.17 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 16 | 0.19 | 0.05 | 0.18 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 15 | 0.2 | 0.03 | 0.2 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 14 | 0.69 | 0.31 | 0.6 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 14 | 0.41 | 0.16 | 0.45 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 14 | 0.26 | 0.11 | 0.22 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 13 | 0.36 | 0.17 | 0.35 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 13 | 0.12 | 0.02 | 0.11 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 12 | 0.28 | 0.04 | 0.27 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 12 | 0.25 | 0.04 | 0.26 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 12 | 0.21 | 0.04 | 0.21 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 11 | 0.25 | 0.1 | 0.22 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 11 | 0.2 | 0.02 | 0.2 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 10 | 0.27 | 0.12 | 0.26 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 10 | 0.27 | 0.12 | 0.26 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 10 | 0.22 | 0.05 | 0.23 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 10 | 0.2 | 0.02 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 10 | 0.2 | 0.02 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 10 | 0.2 | 0.02 | 0.2 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 10 | 0.16 | 0.03 | 0.16 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 10 | 0.16 | 0.03 | 0.16 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 10 | 0.16 | 0.03 | 0.16 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 10 | 0.14 | 0.02 | 0.14 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 9 | 0.66 | 0.32 | 0.62 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 9 | 0.66 | 0.32 | 0.62 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 9 | 0.66 | 0.32 | 0.62 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 9 | 0.18 | 0.02 | 0.18 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 9 | 0.17 | 0.03 | 0.17 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 9 | 0.15 | 0.02 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 9 | 0.15 | 0.02 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 9 | 0.15 | 0.02 | 0.15 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 8 | 1.96 | 0.46 | 1.94 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 8 | 1.96 | 0.46 | 1.94 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 8 | 1.96 | 0.46 | 1.94 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 8 | 1.96 | 0.46 | 1.94 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 8 | 1.96 | 0.46 | 1.94 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 8 | 1.96 | 0.46 | 1.94 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 8 | 0.2 | 0.09 | 0.16 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 8 | 0.15 | 0.03 | 0.15 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 8 | 0.15 | 0.03 | 0.15 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 8 | 0.15 | 0.03 | 0.15 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 8 | 0.13 | 0.02 | 0.13 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 8 | 0.12 | 0.01 | 0.12 |
| (1,849) | 1:105:A:GLN:HG2 | 1:106:A:ARG:H | 7 | 0.36 | 0.15 | 0.39 |
| (1,520) | 1:42:A:GLU:H | 1:42:A:GLU:HB3 | 7 | 0.21 | 0.01 | 0.21 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG21 | 7 | 0.21 | 0.08 | 0.2 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG22 | 7 | 0.21 | 0.08 | 0.2 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG23 | 7 | 0.21 | 0.08 | 0.2 |
| (1,737) | 1:34:A:LYS:H | 1:34:A:LYS:HG2 | 7 | 0.18 | 0.04 | 0.17 |
| (1,640) | 1:74:A:SER:HB2 | 1:75:A:ILE:H | 7 | 0.14 | 0.04 | 0.12 |
| (1,862) | 1:23:A:GLU:HG3 | 1:37:A:THR:HA | 6 | 1.14 | 0.4 | 1.08 |
| (1,899) | 1:79:A:TYR:HB3 | 1:83:A:TYR:HB3 | 6 | 0.98 | 0.44 | 0.96 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG21 | 6 | 0.51 | 0.3 | 0.46 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG22 | 6 | 0.51 | 0.3 | 0.46 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG23 | 6 | 0.51 | 0.3 | 0.46 |
| (1,345) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 6 | 0.44 | 0.16 | 0.5 |
| (1,805) | 1:105:A:GLN:HA | 1:105:A:GLN:HG3 | 6 | 0.32 | 0.04 | 0.33 |
| (1,143) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 6 | 0.25 | 0.06 | 0.26 |
| (1,429) | 1:102:A:GLN:HG3 | 1:103:A:ASN:HD21 | 6 | 0.23 | 0.08 | 0.25 |
| (1,1359) | 1:17:A:TYR:HA | 1:21:A:TRP:HZ2 | 6 | 0.2 | 0.03 | 0.22 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 6 | 0.2 | 0.07 | 0.18 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 6 | 0.2 | 0.07 | 0.18 |
| (1,817) | 1:107:A:LYS:HG2 | 1:107:A:LYS:HE3 | 6 | 0.19 | 0.15 | 0.12 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG21 | 6 | 0.19 | 0.08 | 0.15 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG22 | 6 | 0.19 | 0.08 | 0.15 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG23 | 6 | 0.19 | 0.08 | 0.15 |
| (1,314) | 1:65:A:LYS:HG3 | 1:66:A:VAL:H | 6 | 0.14 | 0.03 | 0.14 |
| (1,546) | 1:71:A:THR:HA | 1:71:A:THR:HB | 6 | 0.12 | 0.0 | 0.12 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG21 | 5 | 1.14 | 0.44 | 1.13 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG22 | 5 | 1.14 | 0.44 | 1.13 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG23 | 5 | 1.14 | 0.44 | 1.13 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG21 | 5 | 1.0 | 0.35 | 1.04 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG22 | 5 | 1.0 | 0.35 | 1.04 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG23 | 5 | 1.0 | 0.35 | 1.04 |
| (1,885) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG3 | 5 | 0.66 | 0.43 | 0.46 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG21 | 5 | 0.53 | 0.33 | 0.51 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG22 | 5 | 0.53 | 0.33 | 0.51 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG23 | 5 | 0.53 | 0.33 | 0.51 |
| (1,504) | 1:14:A:THR:H | 1:14:A:THR:HB | 5 | 0.39 | 0.05 | 0.42 |
| (1,850) | 1:111:A:ARG:HG2 | 1:112:A:ILE:H | 5 | 0.32 | 0.05 | 0.32 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD11 | 5 | 0.27 | 0.06 | 0.3 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD12 | 5 | 0.27 | 0.06 | 0.3 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD13 | 5 | 0.27 | 0.06 | 0.3 |
| (1,198) | 1:49:A:GLU:H | 1:59:A:LEU:H | 5 | 0.24 | 0.07 | 0.24 |
| (1,804) | 1:105:A:GLN:HA | 1:105:A:GLN:HG2 | 5 | 0.22 | 0.03 | 0.21 |
| (1,764) | 1:62:A:MET:HA | 1:62:A:MET:HG3 | 5 | 0.17 | 0.01 | 0.16 |
| (1,795) | 1:99:A:ILE:HA | 1:99:A:ILE:HG12 | 5 | 0.14 | 0.01 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB1 | 1:49:A:GLU:HG3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB2 | 1:49:A:GLU:HG3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB3 | 1:49:A:GLU:HG3 | 5 | 0.13 | 0.02 | 0.14 |
| (1,751) | 1:56:A:GLU:H | 1:56:A:GLU:HG2 | 5 | 0.13 | 0.03 | 0.11 |
| (1,624) | 1:54:A:ARG:HB2 | 1:55:A:GLY:H | 4 | 0.36 | 0.13 | 0.42 |
| (1,763) | 1:62:A:MET:H | 1:62:A:MET:HG3 | 4 | 0.29 | 0.13 | 0.29 |
| (1,810) | 1:107:A:LYS:HA | 1:107:A:LYS:HD3 | 4 | 0.22 | 0.05 | 0.2 |
| (1,871) | 1:51:A:MET:HB2 | 1:54:A:ARG:HG3 | 4 | 0.19 | 0.03 | 0.2 |
| (1,566) | 1:106:A:ARG:H | 1:106:A:ARG:HB2 | 4 | 0.16 | 0.02 | 0.16 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD11 | 4 | 0.16 | 0.02 | 0.16 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD12 | 4 | 0.16 | 0.02 | 0.16 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD13 | 4 | 0.16 | 0.02 | 0.16 |
| (1,1325) | 1:17:A:TYR:HE1 | 1:75:A:ILE:HG12 | 4 | 0.14 | 0.01 | 0.14 |
| (1,1325) | 1:17:A:TYR:HE2 | 1:75:A:ILE:HG12 | 4 | 0.14 | 0.01 | 0.14 |
| (1,826) | 1:115:A:LYS:HA | 1:115:A:LYS:HG3 | 4 | 0.14 | 0.03 | 0.14 |
| (1,354) | 1:54:A:ARG:H | 1:54:A:ARG:HG3 | 4 | 0.13 | 0.01 | 0.13 |
| (1,550) | 1:74:A:SER:H | 1:74:A:SER:HB3 | 4 | 0.12 | 0.02 | 0.11 |
| (1,706) | 1:70:A:SER:HB2 | 1:73:A:GLY:H | 4 | 0.11 | 0.01 | 0.12 |
| (1,809) | 1:107:A:LYS:HA | 1:107:A:LYS:HD2 | 3 | 0.29 | 0.07 | 0.25 |
| (1,886) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG3 | 3 | 0.26 | 0.18 | 0.14 |
| (1,1358) | 1:88:A:SER:HG | 1:100:A:TRP:HD1 | 3 | 0.26 | 0.1 | 0.33 |
| (1,836) | 1:54:A:ARG:HG2 | 1:55:A:GLY:H | 3 | 0.25 | 0.03 | 0.25 |
| (1,679) | 1:116:A:THR:HB | 1:117:A:GLY:H | 3 | 0.24 | 0.04 | 0.22 |
| (1,907) | 1:88:A:SER:HB2 | 1:102:A:GLN:HG3 | 3 | 0.23 | 0.04 | 0.23 |
| (1,846) | 1:78:A:GLN:HE21 | 1:85:A:PRO:HB2 | 3 | 0.23 | 0.03 | 0.21 |
| (1,1281) | 1:99:A:ILE:HD11 | 1:109:A:MET:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,1281) | 1:99:A:ILE:HD12 | 1:109:A:MET:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,1281) | 1:99:A:ILE:HD13 | 1:109:A:MET:H | 3 | 0.2 | 0.01 | 0.2 |
| (1,1094) | 1:46:A:VAL:HG21 | 1:59:A:LEU:H | 3 | 0.19 | 0.04 | 0.21 |
| (1,1094) | 1:46:A:VAL:HG22 | 1:59:A:LEU:H | 3 | 0.19 | 0.04 | 0.21 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1094) | 1:46:A:VAL:HG23 | 1:59:A:LEU:H | 3 | 0.19 | 0.04 | 0.21 |
| (1,938) | 1:75:A:ILE:H | 1:75:A:ILE:HG12 | 3 | 0.18 | 0.05 | 0.15 |
| (1,1055) | 1:38:A:VAL:HG21 | 1:100:A:TRP:HH2 | 3 | 0.17 | 0.01 | 0.17 |
| (1,1055) | 1:38:A:VAL:HG22 | 1:100:A:TRP:HH2 | 3 | 0.17 | 0.01 | 0.17 |
| (1,1055) | 1:38:A:VAL:HG23 | 1:100:A:TRP:HH2 | 3 | 0.17 | 0.01 | 0.17 |
| (1,820) | 1:111:A:ARG:HA | 1:111:A:ARG:HG3 | 3 | 0.16 | 0.03 | 0.15 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD21 | 3 | 0.16 | 0.01 | 0.16 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD22 | 3 | 0.16 | 0.01 | 0.16 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD23 | 3 | 0.16 | 0.01 | 0.16 |
| (1,531) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 3 | 0.16 | 0.01 | 0.16 |
| (1,818) | 1:107:A:LYS:HG3 | 1:107:A:LYS:HE3 | 3 | 0.14 | 0.04 | 0.14 |
| (1,413) | 1:78:A:GLN:HE21 | 1:85:A:PRO:HB3 | 3 | 0.12 | 0.02 | 0.13 |
| (1,415) | 1:78:A:GLN:HE22 | 1:85:A:PRO:HB2 | 3 | 0.12 | 0.01 | 0.12 |
| (1,674) | 1:110:A:THR:HB | 1:111:A:ARG:H | 3 | 0.12 | 0.0 | 0.12 |
| (1,940) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG2 | 2 | 0.73 | 0.62 | 0.73 |
| (1,733) | 1:23:A:GLU:HA | 1:23:A:GLU:HG2 | 2 | 0.56 | 0.12 | 0.56 |
| (1,766) | 1:65:A:LYS:H | 1:65:A:LYS:HG3 | 2 | 0.42 | 0.14 | 0.42 |
| (1,792) | 1:92:A:ARG:HB2 | 1:92:A:ARG:HD3 | 2 | 0.34 | 0.01 | 0.34 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG11 | 2 | 0.3 | 0.02 | 0.3 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG12 | 2 | 0.3 | 0.02 | 0.3 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG13 | 2 | 0.3 | 0.02 | 0.3 |
| (1,503) | 1:13:A:GLU:H | 1:13:A:GLU:HB2 | 2 | 0.29 | 0.04 | 0.29 |
| (1,1049) | 1:38:A:VAL:HG21 | 1:47:A:GLU:HB2 | 2 | 0.24 | 0.03 | 0.24 |
| (1,1049) | 1:38:A:VAL:HG22 | 1:47:A:GLU:HB2 | 2 | 0.24 | 0.03 | 0.24 |
| (1,1049) | 1:38:A:VAL:HG23 | 1:47:A:GLU:HB2 | 2 | 0.24 | 0.03 | 0.24 |
| (1,906) | 1:88:A:SER:HB2 | 1:102:A:GLN:HG2 | 2 | 0.22 | 0.02 | 0.22 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG21 | 2 | 0.22 | 0.02 | 0.22 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG22 | 2 | 0.22 | 0.02 | 0.22 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG23 | 2 | 0.22 | 0.02 | 0.22 |
| (1,739) | 1:34:A:LYS:H | 1:34:A:LYS:HG3 | 2 | 0.2 | 0.02 | 0.2 |
| (1,835) | 1:47:A:GLU:HG2 | 1:48:A:THR:H | 2 | 0.2 | 0.02 | 0.2 |
| (1,219) | 1:118:A:ARG:H | 1:119:A:GLU:H | 2 | 0.18 | 0.0 | 0.18 |
| (1,400) | 1:29:A:PRO:HG2 | 1:32:A:GLY:H | 2 | 0.18 | 0.0 | 0.18 |
| (1,400) | 1:29:A:PRO:HG3 | 1:32:A:GLY:H | 2 | 0.18 | 0.0 | 0.18 |
| (1,684) | 1:121:A:LYS:HB2 | 1:122:A:ASP:H | 2 | 0.18 | 0.03 | 0.18 |
| (1,734) | 1:23:A:GLU:HA | 1:23:A:GLU:HG3 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1327) | 1:21:A:TRP:HA | 1:21:A:TRP:HE3 | 2 | 0.15 | 0.04 | 0.15 |
| (1,814) | 1:107:A:LYS:HG3 | 1:107:A:LYS:HE2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,641) | 1:74:A:SER:HB3 | 1:75:A:ILE:H | 2 | 0.14 | 0.02 | 0.14 |
| (1,913) | 1:89:A:THR:HB | 1:101:A:GLU:HB2 | 2 | 0.13 | 0.02 | 0.13 |
| (1,669) | 1:103:A:ASN:HA | 1:104:A:GLY:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,625) | 1:54:A:ARG:HB3 | 1:55:A:GLY:H | 2 | 0.12 | 0.0 | 0.12 |

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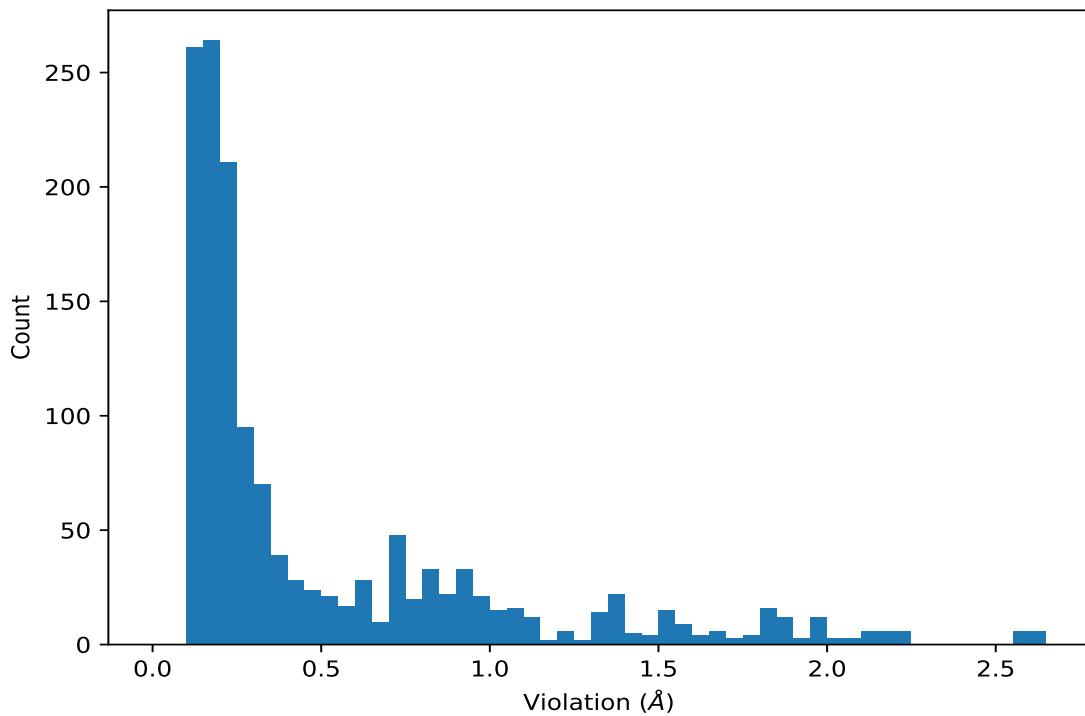
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|---------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,861) | 1:65:A:LYS:HG2 | 1:66:A:VAL:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,567) | 1:106:A:ARG:H | 1:106:A:ARG:HB3 | 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 [\(i\)](#)

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 7 | 2.65 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 7 | 2.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 7 | 2.65 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 7 | 2.65 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 7 | 2.65 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 7 | 2.65 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 18 | 2.57 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 18 | 2.57 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 18 | 2.57 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 18 | 2.57 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 18 | 2.57 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 18 | 2.57 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 14 | 2.22 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 14 | 2.22 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 14 | 2.22 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 18 | 2.22 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 18 | 2.22 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 18 | 2.22 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 2 | 2.15 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 2 | 2.15 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 2 | 2.15 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 2 | 2.15 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 2 | 2.15 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 2 | 2.15 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 13 | 2.13 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 13 | 2.13 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 13 | 2.13 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 4 | 2.12 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 4 | 2.12 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 4 | 2.12 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 10 | 2.08 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 10 | 2.08 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 10 | 2.08 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 9 | 2.04 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 9 | 2.04 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 9 | 2.04 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 7 | 1.99 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 7 | 1.99 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 7 | 1.99 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 16 | 1.98 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 16 | 1.98 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 16 | 1.98 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 16 | 1.98 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 16 | 1.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 16 | 1.98 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 6 | 1.95 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 6 | 1.95 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 6 | 1.95 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 2 | 1.92 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 2 | 1.92 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 2 | 1.92 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 4 | 1.89 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 4 | 1.89 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 4 | 1.89 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 4 | 1.89 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 4 | 1.89 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 4 | 1.89 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 8 | 1.89 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 8 | 1.89 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 8 | 1.89 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 16 | 1.85 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 16 | 1.85 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 16 | 1.85 |
| (1,862) | 1:23:A:GLU:HG3 | 1:37:A:THR:HA | 15 | 1.83 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 17 | 1.82 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 17 | 1.82 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 17 | 1.82 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 1 | 1.81 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 1 | 1.81 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 1 | 1.81 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 1 | 1.81 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 1 | 1.81 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 1 | 1.81 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 5 | 1.81 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 5 | 1.81 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 5 | 1.81 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 11 | 1.8 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 11 | 1.8 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 11 | 1.8 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 8 | 1.79 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 19 | 1.78 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 19 | 1.78 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 19 | 1.78 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 15 | 1.71 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 15 | 1.71 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 15 | 1.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG21 | 19 | 1.67 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG22 | 19 | 1.67 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG23 | 19 | 1.67 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 1 | 1.67 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 11 | 1.67 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 16 | 1.65 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 13 | 1.63 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 17 | 1.61 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 10 | 1.6 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 12 | 1.6 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 3 | 1.59 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 2 | 1.57 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 15 | 1.57 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 18 | 1.57 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 20 | 1.57 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 14 | 1.56 |
| (1,899) | 1:79:A:TYR:HB3 | 1:83:A:TYR:HB3 | 11 | 1.55 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 6 | 1.55 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 19 | 1.55 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 9 | 1.54 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 12 | 1.53 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 12 | 1.53 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 12 | 1.53 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 1 | 1.53 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG21 | 8 | 1.52 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG22 | 8 | 1.52 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG23 | 8 | 1.52 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 5 | 1.52 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 7 | 1.52 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 20 | 1.52 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 20 | 1.51 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 20 | 1.51 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 20 | 1.51 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 8 | 1.5 |
| (1,757) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 4 | 1.49 |
| (1,899) | 1:79:A:TYR:HB3 | 1:83:A:TYR:HB3 | 1 | 1.48 |
| (1,885) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG3 | 10 | 1.48 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 5 | 1.46 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 3 | 1.44 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 3 | 1.44 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 3 | 1.44 |
| (1,862) | 1:23:A:GLU:HG3 | 1:37:A:THR:HA | 1 | 1.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 6 | 1.4 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 11 | 1.38 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG21 | 19 | 1.38 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG22 | 19 | 1.38 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG23 | 19 | 1.38 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 4 | 1.37 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG21 | 8 | 1.37 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG22 | 8 | 1.37 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG23 | 8 | 1.37 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 13 | 1.37 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 15 | 1.37 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 17 | 1.37 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 14 | 1.36 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 8 | 1.35 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 8 | 1.35 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 8 | 1.35 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 8 | 1.35 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 8 | 1.35 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 8 | 1.35 |
| (1,940) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG2 | 3 | 1.35 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 3 | 1.35 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 10 | 1.35 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 16 | 1.35 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 18 | 1.34 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 9 | 1.33 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG21 | 10 | 1.32 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG22 | 10 | 1.32 |
| (1,1129) | 1:65:A:LYS:HE2 | 1:67:A:ILE:HG23 | 10 | 1.32 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG21 | 10 | 1.32 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG22 | 10 | 1.32 |
| (1,1129) | 1:65:A:LYS:HE3 | 1:67:A:ILE:HG23 | 10 | 1.32 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 2 | 1.32 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 7 | 1.32 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 11 | 1.31 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 11 | 1.31 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 11 | 1.31 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 12 | 1.3 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 19 | 1.28 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 1 | 1.25 |
| (1,1111) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 1 | 1.24 |
| (1,1111) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 1 | 1.24 |
| (1,1111) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 1 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 14 | 1.22 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 14 | 1.22 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 14 | 1.22 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 8 | 1.16 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 8 | 1.16 |
| (1,862) | 1:23:A:GLU:HG3 | 1:37:A:THR:HA | 3 | 1.14 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 13 | 1.13 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 13 | 1.13 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG21 | 18 | 1.13 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG22 | 18 | 1.13 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG23 | 18 | 1.13 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 14 | 1.1 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 14 | 1.1 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 14 | 1.1 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 14 | 1.1 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 14 | 1.1 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 14 | 1.1 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 8 | 1.09 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 13 | 1.09 |
| (1,899) | 1:79:A:TYR:HB3 | 1:83:A:TYR:HB3 | 20 | 1.08 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 13 | 1.08 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 6 | 1.07 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 5 | 1.05 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 5 | 1.05 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG21 | 6 | 1.05 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG22 | 6 | 1.05 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG23 | 6 | 1.05 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 8 | 1.05 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 8 | 1.05 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 8 | 1.05 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 8 | 1.05 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 11 | 1.05 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 17 | 1.05 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 2 | 1.04 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 2 | 1.04 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG21 | 18 | 1.04 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG22 | 18 | 1.04 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG23 | 18 | 1.04 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 10 | 1.03 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 10 | 1.03 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 18 | 1.03 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 18 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 18 | 1.03 |
| (1,862) | 1:23:A:GLU:HG3 | 1:37:A:THR:HA | 9 | 1.03 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 3 | 1.02 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 3 | 1.02 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 5 | 1.02 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 17 | 1.02 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 18 | 0.99 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 18 | 0.99 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 19 | 0.99 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 19 | 0.99 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 2 | 0.99 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG21 | 10 | 0.98 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG22 | 10 | 0.98 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG23 | 10 | 0.98 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 18 | 0.97 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 18 | 0.97 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 18 | 0.97 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 18 | 0.97 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 18 | 0.97 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 18 | 0.97 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 14 | 0.97 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 15 | 0.97 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 11 | 0.96 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 11 | 0.96 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 17 | 0.95 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 17 | 0.95 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 10 | 0.95 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 9 | 0.94 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 9 | 0.94 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 12 | 0.94 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 12 | 0.94 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 3 | 0.94 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 3 | 0.94 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 7 | 0.94 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 19 | 0.94 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 2 | 0.93 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 12 | 0.93 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 16 | 0.92 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 16 | 0.92 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG21 | 19 | 0.92 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG22 | 19 | 0.92 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG23 | 19 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 10 | 0.92 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 6 | 0.91 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 6 | 0.91 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 18 | 0.91 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 19 | 0.91 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 16 | 0.91 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 8 | 0.9 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 8 | 0.9 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 8 | 0.9 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 8 | 0.9 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 8 | 0.9 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 8 | 0.9 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 4 | 0.9 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 4 | 0.9 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 4 | 0.9 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 16 | 0.9 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 16 | 0.9 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 16 | 0.9 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 14 | 0.89 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 14 | 0.89 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 15 | 0.89 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 15 | 0.89 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 20 | 0.89 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 20 | 0.89 |
| (1,554) | 1:84:A:TYR:HA | 1:85:A:PRO:HA | 9 | 0.89 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 3 | 0.88 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 3 | 0.88 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 3 | 0.88 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 7 | 0.86 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 7 | 0.86 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 13 | 0.86 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 13 | 0.86 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 13 | 0.86 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 4 | 0.85 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 4 | 0.85 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 4 | 0.85 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 4 | 0.85 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 4 | 0.85 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 4 | 0.85 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 9 | 0.85 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG21 | 10 | 0.84 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG22 | 10 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG23 | 10 | 0.84 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 11 | 0.84 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 11 | 0.84 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 11 | 0.84 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 8 | 0.84 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 8 | 0.84 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 8 | 0.84 |
| (1,899) | 1:79:A:TYR:HB3 | 1:83:A:TYR:HB3 | 5 | 0.84 |
| (1,862) | 1:23:A:GLU:HG3 | 1:37:A:THR:HA | 16 | 0.84 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 1 | 0.83 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 1 | 0.83 |
| (1,1489) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 4 | 0.83 |
| (1,1489) | 1:58:A:GLN:HG3 | 1:59:A:LEU:H | 4 | 0.83 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 13 | 0.83 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 13 | 0.83 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 13 | 0.83 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 13 | 0.83 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 13 | 0.83 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 13 | 0.83 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 11 | 0.83 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 17 | 0.83 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 12 | 0.82 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 10 | 0.81 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 10 | 0.81 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 10 | 0.81 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 16 | 0.8 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 16 | 0.8 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 16 | 0.8 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 16 | 0.8 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 16 | 0.8 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 16 | 0.8 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 6 | 0.79 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 5 | 0.79 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 10 | 0.78 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 10 | 0.78 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 10 | 0.78 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 10 | 0.78 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 10 | 0.78 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 10 | 0.78 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 16 | 0.78 |
| (1,306) | 1:74:A:SER:HA | 1:92:A:ARG:H | 9 | 0.78 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 6 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 17 | 0.77 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 17 | 0.77 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 17 | 0.77 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 20 | 0.77 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 2 | 0.76 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 2 | 0.76 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 2 | 0.76 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 14 | 0.75 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 15 | 0.75 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 11 | 0.74 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 11 | 0.74 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 11 | 0.74 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 11 | 0.74 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 11 | 0.74 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 11 | 0.74 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 7 | 0.74 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 7 | 0.74 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 7 | 0.74 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 1 | 0.73 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 1 | 0.73 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 1 | 0.73 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 9 | 0.73 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 9 | 0.73 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 9 | 0.73 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 7 | 0.72 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 2 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 7 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 7 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 7 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 7 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 7 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 7 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 9 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 9 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 9 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 9 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 9 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 9 | 0.71 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 17 | 0.7 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 17 | 0.7 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 17 | 0.7 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 17 | 0.7 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 17 | 0.7 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 17 | 0.7 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG21 | 18 | 0.7 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG22 | 18 | 0.7 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG23 | 18 | 0.7 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 15 | 0.7 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 15 | 0.7 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 15 | 0.7 |
| (1,885) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG3 | 15 | 0.7 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 8 | 0.7 |
| (1,939) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG2 | 10 | 0.69 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 4 | 0.69 |
| (1,733) | 1:23:A:GLU:HA | 1:23:A:GLU:HG2 | 1 | 0.69 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 5 | 0.67 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 5 | 0.67 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 5 | 0.67 |
| (1,755) | 1:58:A:GLN:HG2 | 1:59:A:LEU:H | 1 | 0.65 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG21 | 10 | 0.65 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG22 | 10 | 0.65 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG23 | 10 | 0.65 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 4 | 0.64 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 5 | 0.63 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 5 | 0.63 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 5 | 0.63 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 5 | 0.63 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 5 | 0.63 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 5 | 0.63 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 2 | 0.62 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 2 | 0.62 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 2 | 0.62 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 6 | 0.61 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 6 | 0.61 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 6 | 0.61 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 15 | 0.61 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 15 | 0.61 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 15 | 0.61 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 20 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,345) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 9 | 0.61 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 6 | 0.6 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 6 | 0.6 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 6 | 0.6 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 6 | 0.6 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 6 | 0.6 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 6 | 0.6 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG21 | 8 | 0.6 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG22 | 8 | 0.6 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG23 | 8 | 0.6 |
| (1,862) | 1:23:A:GLU:HG3 | 1:37:A:THR:HA | 13 | 0.6 |
| (1,849) | 1:105:A:GLN:HG2 | 1:106:A:ARG:H | 17 | 0.59 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 14 | 0.59 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 18 | 0.59 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 11 | 0.57 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 15 | 0.56 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 15 | 0.56 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 15 | 0.56 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 15 | 0.56 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 15 | 0.56 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 15 | 0.56 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 12 | 0.56 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 12 | 0.56 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 12 | 0.56 |
| (1,899) | 1:79:A:TYR:HB3 | 1:83:A:TYR:HB3 | 8 | 0.56 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 16 | 0.56 |
| (1,766) | 1:65:A:LYS:H | 1:65:A:LYS:HG3 | 9 | 0.55 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 10 | 0.55 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG21 | 16 | 0.54 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG22 | 16 | 0.54 |
| (1,500) | 1:98:A:LEU:H | 1:108:A:THR:HG23 | 16 | 0.54 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 3 | 0.53 |
| (1,345) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 15 | 0.53 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 1 | 0.52 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 1 | 0.52 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 1 | 0.52 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 1 | 0.52 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 1 | 0.52 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 1 | 0.52 |
| (1,886) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG3 | 10 | 0.52 |
| (1,817) | 1:107:A:LYS:HG2 | 1:107:A:LYS:HE3 | 18 | 0.52 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 2 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG21 | 8 | 0.51 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG22 | 8 | 0.51 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG23 | 8 | 0.51 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 12 | 0.5 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 17 | 0.5 |
| (1,345) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 1 | 0.5 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 20 | 0.5 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 19 | 0.49 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 19 | 0.49 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 19 | 0.49 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 19 | 0.49 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 19 | 0.49 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 19 | 0.49 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 19 | 0.49 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 19 | 0.49 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 19 | 0.49 |
| (1,345) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 20 | 0.49 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 16 | 0.49 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 9 | 0.49 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 3 | 0.48 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 17 | 0.46 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 17 | 0.46 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 17 | 0.46 |
| (1,885) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG3 | 18 | 0.46 |
| (1,849) | 1:105:A:GLN:HG2 | 1:106:A:ARG:H | 16 | 0.46 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 12 | 0.46 |
| (1,624) | 1:54:A:ARG:HB2 | 1:55:A:GLY:H | 20 | 0.46 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 7 | 0.45 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 7 | 0.45 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 6 | 0.45 |
| (1,624) | 1:54:A:ARG:HB2 | 1:55:A:GLY:H | 2 | 0.45 |
| (1,763) | 1:62:A:MET:H | 1:62:A:MET:HG3 | 6 | 0.44 |
| (1,733) | 1:23:A:GLU:HA | 1:23:A:GLU:HG2 | 13 | 0.44 |
| (1,345) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 5 | 0.44 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 13 | 0.43 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 13 | 0.43 |
| (1,504) | 1:14:A:THR:H | 1:14:A:THR:HB | 14 | 0.43 |
| (1,344) | 1:23:A:GLU:H | 1:23:A:GLU:HG2 | 1 | 0.43 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 9 | 0.43 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 20 | 0.43 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG21 | 16 | 0.42 |
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG22 | 16 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1320) | 1:97:A:THR:HB | 1:108:A:THR:HG23 | 16 | 0.42 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 7 | 0.42 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 7 | 0.42 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 7 | 0.42 |
| (1,504) | 1:14:A:THR:H | 1:14:A:THR:HB | 5 | 0.42 |
| (1,504) | 1:14:A:THR:H | 1:14:A:THR:HB | 8 | 0.42 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 12 | 0.41 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 12 | 0.41 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 12 | 0.41 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 14 | 0.41 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 9 | 0.4 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 9 | 0.4 |
| (1,849) | 1:105:A:GLN:HG2 | 1:106:A:ARG:H | 14 | 0.4 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 14 | 0.4 |
| (1,735) | 1:23:A:GLU:HB2 | 1:23:A:GLU:HG3 | 1 | 0.4 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 19 | 0.4 |
| (1,504) | 1:14:A:THR:H | 1:14:A:THR:HB | 6 | 0.4 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 12 | 0.39 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 12 | 0.39 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 12 | 0.39 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 12 | 0.39 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 12 | 0.39 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 12 | 0.39 |
| (1,849) | 1:105:A:GLN:HG2 | 1:106:A:ARG:H | 1 | 0.39 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 6 | 0.39 |
| (1,763) | 1:62:A:MET:H | 1:62:A:MET:HG3 | 9 | 0.39 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 18 | 0.39 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 13 | 0.38 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 17 | 0.38 |
| (1,809) | 1:107:A:LYS:HA | 1:107:A:LYS:HD2 | 10 | 0.38 |
| (1,624) | 1:54:A:ARG:HB2 | 1:55:A:GLY:H | 13 | 0.38 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 18 | 0.38 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 17 | 0.38 |
| (1,899) | 1:79:A:TYR:HB3 | 1:83:A:TYR:HB3 | 17 | 0.37 |
| (1,850) | 1:111:A:ARG:HG2 | 1:112:A:ILE:H | 8 | 0.37 |
| (1,850) | 1:111:A:ARG:HG2 | 1:112:A:ILE:H | 9 | 0.37 |
| (1,805) | 1:105:A:GLN:HA | 1:105:A:GLN:HG3 | 1 | 0.37 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 2 | 0.37 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 10 | 0.37 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG21 | 17 | 0.36 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG22 | 17 | 0.36 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG23 | 17 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 12 | 0.36 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 3 | 0.36 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 12 | 0.36 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 17 | 0.36 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 13 | 0.36 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG21 | 1 | 0.35 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG22 | 1 | 0.35 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG23 | 1 | 0.35 |
| (1,849) | 1:105:A:GLN:HG2 | 1:106:A:ARG:H | 3 | 0.35 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 6 | 0.35 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 15 | 0.35 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 16 | 0.35 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 1 | 0.35 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 15 | 0.35 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 3 | 0.34 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 3 | 0.34 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 3 | 0.34 |
| (1,1108) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 20 | 0.34 |
| (1,1108) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 20 | 0.34 |
| (1,1108) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 20 | 0.34 |
| (1,885) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG3 | 7 | 0.34 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 9 | 0.34 |
| (1,805) | 1:105:A:GLN:HA | 1:105:A:GLN:HG3 | 14 | 0.34 |
| (1,805) | 1:105:A:GLN:HA | 1:105:A:GLN:HG3 | 16 | 0.34 |
| (1,792) | 1:92:A:ARG:HB2 | 1:92:A:ARG:HD3 | 14 | 0.34 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 9 | 0.34 |
| (1,429) | 1:102:A:GLN:HG3 | 1:103:A:ASN:HD21 | 12 | 0.34 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 5 | 0.34 |
| (1,198) | 1:49:A:GLU:H | 1:59:A:LEU:H | 5 | 0.34 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 20 | 0.33 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 20 | 0.33 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 20 | 0.33 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 20 | 0.33 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 20 | 0.33 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 20 | 0.33 |
| (1,1358) | 1:88:A:SER:HG | 1:100:A:TRP:HD1 | 5 | 0.33 |
| (1,1358) | 1:88:A:SER:HG | 1:100:A:TRP:HD1 | 7 | 0.33 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG21 | 18 | 0.33 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG22 | 18 | 0.33 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG23 | 18 | 0.33 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 3 | 0.33 |
| (1,792) | 1:92:A:ARG:HB2 | 1:92:A:ARG:HD3 | 6 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 1 | 0.33 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 4 | 0.33 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG2 | 3 | 0.32 |
| (1,1448) | 1:46:A:VAL:HG21 | 1:58:A:GLN:HG3 | 3 | 0.32 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG2 | 3 | 0.32 |
| (1,1448) | 1:46:A:VAL:HG22 | 1:58:A:GLN:HG3 | 3 | 0.32 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG2 | 3 | 0.32 |
| (1,1448) | 1:46:A:VAL:HG23 | 1:58:A:GLN:HG3 | 3 | 0.32 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 16 | 0.32 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 16 | 0.32 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG11 | 1 | 0.32 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG12 | 1 | 0.32 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG13 | 1 | 0.32 |
| (1,850) | 1:111:A:ARG:HG2 | 1:112:A:ILE:H | 12 | 0.32 |
| (1,805) | 1:105:A:GLN:HA | 1:105:A:GLN:HG3 | 17 | 0.32 |
| (1,805) | 1:105:A:GLN:HA | 1:105:A:GLN:HG3 | 20 | 0.32 |
| (1,503) | 1:13:A:GLU:H | 1:13:A:GLU:HB2 | 9 | 0.32 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 20 | 0.32 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 20 | 0.32 |
| (1,143) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 18 | 0.32 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD11 | 6 | 0.31 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD12 | 6 | 0.31 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD13 | 6 | 0.31 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD11 | 19 | 0.31 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD12 | 19 | 0.31 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD13 | 19 | 0.31 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 6 | 0.31 |
| (1,847) | 1:91:A:LYS:HG2 | 1:92:A:ARG:H | 10 | 0.31 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 5 | 0.31 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 18 | 0.31 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 19 | 0.31 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 19 | 0.31 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 18 | 0.3 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 18 | 0.3 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD11 | 17 | 0.3 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD12 | 17 | 0.3 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD13 | 17 | 0.3 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 2 | 0.3 |
| (1,885) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG3 | 11 | 0.3 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 17 | 0.3 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 5 | 0.3 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 14 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 6 | 0.29 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 6 | 0.29 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 12 | 0.29 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 12 | 0.29 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD11 | 4 | 0.29 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD12 | 4 | 0.29 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD13 | 4 | 0.29 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 3 | 0.29 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 20 | 0.29 |
| (1,850) | 1:111:A:ARG:HG2 | 1:112:A:ILE:H | 16 | 0.29 |
| (1,810) | 1:107:A:LYS:HA | 1:107:A:LYS:HD3 | 4 | 0.29 |
| (1,679) | 1:116:A:THR:HB | 1:117:A:GLY:H | 2 | 0.29 |
| (1,504) | 1:14:A:THR:H | 1:14:A:THR:HB | 12 | 0.29 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 13 | 0.29 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 15 | 0.29 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 15 | 0.29 |
| (1,143) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 12 | 0.29 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 12 | 0.28 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 12 | 0.28 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG11 | 2 | 0.28 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG12 | 2 | 0.28 |
| (1,1046) | 1:23:A:GLU:HG2 | 1:38:A:VAL:HG13 | 2 | 0.28 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 7 | 0.28 |
| (1,907) | 1:88:A:SER:HB2 | 1:102:A:GLN:HG3 | 10 | 0.28 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 17 | 0.28 |
| (1,836) | 1:54:A:ARG:HG2 | 1:55:A:GLY:H | 4 | 0.28 |
| (1,804) | 1:105:A:GLN:HA | 1:105:A:GLN:HG2 | 3 | 0.28 |
| (1,766) | 1:65:A:LYS:H | 1:65:A:LYS:HG3 | 18 | 0.28 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 9 | 0.28 |
| (1,511) | 1:23:A:GLU:HA | 1:23:A:GLU:HB3 | 1 | 0.28 |
| (1,429) | 1:102:A:GLN:HG3 | 1:103:A:ASN:HD21 | 7 | 0.28 |
| (1,429) | 1:102:A:GLN:HG3 | 1:103:A:ASN:HD21 | 17 | 0.28 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 11 | 0.28 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 13 | 0.28 |
| (1,1049) | 1:38:A:VAL:HG21 | 1:47:A:GLU:HB2 | 6 | 0.27 |
| (1,1049) | 1:38:A:VAL:HG22 | 1:47:A:GLU:HB2 | 6 | 0.27 |
| (1,1049) | 1:38:A:VAL:HG23 | 1:47:A:GLU:HB2 | 6 | 0.27 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 17 | 0.27 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 5 | 0.27 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 6 | 0.27 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 14 | 0.27 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 10 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 14 | 0.27 |
| (1,846) | 1:78:A:GLN:HE21 | 1:85:A:PRO:HB2 | 7 | 0.27 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 7 | 0.27 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 8 | 0.27 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 12 | 0.27 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 19 | 0.27 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 4 | 0.27 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 1 | 0.27 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 6 | 0.27 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 10 | 0.27 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 4 | 0.26 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 8 | 0.26 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 17 | 0.26 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 10 | 0.26 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 11 | 0.26 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 14 | 0.26 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 8 | 0.26 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 16 | 0.26 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 4 | 0.26 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 7 | 0.26 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 7 | 0.26 |
| (1,333) | 1:101:A:GLU:HG3 | 1:102:A:GLN:H | 11 | 0.26 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 1 | 0.26 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 9 | 0.26 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 18 | 0.26 |
| (1,143) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 20 | 0.26 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 6 | 0.25 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 6 | 0.25 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 19 | 0.25 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 19 | 0.25 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG21 | 13 | 0.25 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG22 | 13 | 0.25 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG23 | 13 | 0.25 |
| (1,938) | 1:75:A:ILE:H | 1:75:A:ILE:HG12 | 1 | 0.25 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 15 | 0.25 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 3 | 0.25 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 13 | 0.25 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 16 | 0.25 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 18 | 0.25 |
| (1,850) | 1:111:A:ARG:HG2 | 1:112:A:ILE:H | 11 | 0.25 |
| (1,836) | 1:54:A:ARG:HG2 | 1:55:A:GLY:H | 1 | 0.25 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 9 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 4 | 0.25 |
| (1,809) | 1:107:A:LYS:HA | 1:107:A:LYS:HD2 | 6 | 0.25 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 10 | 0.25 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 15 | 0.25 |
| (1,737) | 1:34:A:LYS:H | 1:34:A:LYS:HG2 | 16 | 0.25 |
| (1,686) | 1:122:A:ASP:HB3 | 1:123:A:GLU:H | 8 | 0.25 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 11 | 0.25 |
| (1,503) | 1:13:A:GLU:H | 1:13:A:GLU:HB2 | 1 | 0.25 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 17 | 0.25 |
| (1,321) | 1:86:A:LEU:HG | 1:87:A:LYS:H | 10 | 0.25 |
| (1,143) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 16 | 0.25 |
| (1,1359) | 1:17:A:TYR:HA | 1:21:A:TRP:HZ2 | 13 | 0.24 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG21 | 19 | 0.24 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG22 | 19 | 0.24 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG23 | 19 | 0.24 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG21 | 4 | 0.24 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG22 | 4 | 0.24 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG23 | 4 | 0.24 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG21 | 13 | 0.24 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG22 | 13 | 0.24 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG23 | 13 | 0.24 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 14 | 0.24 |
| (1,906) | 1:88:A:SER:HB2 | 1:102:A:GLN:HG2 | 7 | 0.24 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 2 | 0.24 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 10 | 0.24 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 11 | 0.24 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 2 | 0.24 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 4 | 0.24 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 7 | 0.24 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 12 | 0.24 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 15 | 0.24 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 4 | 0.24 |
| (1,520) | 1:42:A:GLU:H | 1:42:A:GLU:HB3 | 6 | 0.24 |
| (1,374) | 1:105:A:GLN:H | 1:105:A:GLN:HG3 | 1 | 0.24 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 6 | 0.24 |
| (1,198) | 1:49:A:GLU:H | 1:59:A:LEU:H | 1 | 0.24 |
| (1,198) | 1:49:A:GLU:H | 1:59:A:LEU:H | 6 | 0.24 |
| (1,198) | 1:49:A:GLU:H | 1:59:A:LEU:H | 11 | 0.24 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 2 | 0.23 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 2 | 0.23 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 6 | 0.23 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG21 | 16 | 0.23 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG22 | 16 | 0.23 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG23 | 16 | 0.23 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 1 | 0.23 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 1 | 0.23 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 1 | 0.23 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 18 | 0.23 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 18 | 0.23 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 18 | 0.23 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG21 | 8 | 0.23 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG22 | 8 | 0.23 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG23 | 8 | 0.23 |
| (1,933) | 1:21:A:TRP:HA | 1:112:A:ILE:HG13 | 7 | 0.23 |
| (1,915) | 1:90:A:LEU:HG | 1:100:A:TRP:HD1 | 1 | 0.23 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 19 | 0.23 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 19 | 0.23 |
| (1,907) | 1:88:A:SER:HB2 | 1:102:A:GLN:HG3 | 13 | 0.23 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 12 | 0.23 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 15 | 0.23 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 20 | 0.23 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 8 | 0.23 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 9 | 0.23 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 11 | 0.23 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 11 | 0.23 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 7 | 0.23 |
| (1,809) | 1:107:A:LYS:HA | 1:107:A:LYS:HD2 | 4 | 0.23 |
| (1,805) | 1:105:A:GLN:HA | 1:105:A:GLN:HG3 | 3 | 0.23 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 1 | 0.23 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 16 | 0.23 |
| (1,520) | 1:42:A:GLU:H | 1:42:A:GLU:HB3 | 8 | 0.23 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 2 | 0.23 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 13 | 0.23 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 19 | 0.23 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 20 | 0.23 |
| (1,143) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 2 | 0.23 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 17 | 0.22 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 17 | 0.22 |
| (1,1359) | 1:17:A:TYR:HA | 1:21:A:TRP:HZ2 | 7 | 0.22 |
| (1,1359) | 1:17:A:TYR:HA | 1:21:A:TRP:HZ2 | 18 | 0.22 |
| (1,1281) | 1:99:A:ILE:HD11 | 1:109:A:MET:H | 9 | 0.22 |
| (1,1281) | 1:99:A:ILE:HD12 | 1:109:A:MET:H | 9 | 0.22 |
| (1,1281) | 1:99:A:ILE:HD13 | 1:109:A:MET:H | 9 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1094) | 1:46:A:VAL:HG21 | 1:59:A:LEU:H | 14 | 0.22 |
| (1,1094) | 1:46:A:VAL:HG22 | 1:59:A:LEU:H | 14 | 0.22 |
| (1,1094) | 1:46:A:VAL:HG23 | 1:59:A:LEU:H | 14 | 0.22 |
| (1,924) | 1:101:A:GLU:HG2 | 1:106:A:ARG:HG2 | 19 | 0.22 |
| (1,924) | 1:101:A:GLU:HG2 | 1:106:A:ARG:HG3 | 19 | 0.22 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 1 | 0.22 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 3 | 0.22 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 5 | 0.22 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 6 | 0.22 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 13 | 0.22 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 17 | 0.22 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 18 | 0.22 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 18 | 0.22 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 1 | 0.22 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 19 | 0.22 |
| (1,871) | 1:51:A:MET:HB2 | 1:54:A:ARG:HG3 | 2 | 0.22 |
| (1,863) | 1:21:A:TRP:H | 1:37:A:THR:HB | 6 | 0.22 |
| (1,835) | 1:47:A:GLU:HG2 | 1:48:A:THR:H | 1 | 0.22 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 2 | 0.22 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 16 | 0.22 |
| (1,804) | 1:105:A:GLN:HA | 1:105:A:GLN:HG2 | 17 | 0.22 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 2 | 0.22 |
| (1,739) | 1:34:A:LYS:H | 1:34:A:LYS:HG3 | 6 | 0.22 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 5 | 0.22 |
| (1,679) | 1:116:A:THR:HB | 1:117:A:GLY:H | 19 | 0.22 |
| (1,640) | 1:74:A:SER:HB2 | 1:75:A:ILE:H | 7 | 0.22 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 10 | 0.22 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 19 | 0.22 |
| (1,429) | 1:102:A:GLN:HG3 | 1:103:A:ASN:HD21 | 13 | 0.22 |
| (1,391) | 1:102:A:GLN:HG2 | 1:102:A:GLN:HE22 | 4 | 0.22 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 10 | 0.22 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 18 | 0.22 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 10 | 0.22 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 14 | 0.22 |
| (1,1359) | 1:17:A:TYR:HA | 1:21:A:TRP:HZ2 | 2 | 0.21 |
| (1,1094) | 1:46:A:VAL:HG21 | 1:59:A:LEU:H | 13 | 0.21 |
| (1,1094) | 1:46:A:VAL:HG22 | 1:59:A:LEU:H | 13 | 0.21 |
| (1,1094) | 1:46:A:VAL:HG23 | 1:59:A:LEU:H | 13 | 0.21 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 18 | 0.21 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 18 | 0.21 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 18 | 0.21 |
| (1,1049) | 1:38:A:VAL:HG21 | 1:47:A:GLU:HB2 | 10 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1049) | 1:38:A:VAL:HG22 | 1:47:A:GLU:HB2 | 10 | 0.21 |
| (1,1049) | 1:38:A:VAL:HG23 | 1:47:A:GLU:HB2 | 10 | 0.21 |
| (1,918) | 1:94:A:GLU:HB2 | 1:95:A:ASN:HD22 | 16 | 0.21 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 7 | 0.21 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 11 | 0.21 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 12 | 0.21 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 8 | 0.21 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 17 | 0.21 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 18 | 0.21 |
| (1,865) | 1:18:A:TYR:HA | 1:40:A:PHE:HB3 | 14 | 0.21 |
| (1,846) | 1:78:A:GLN:HE21 | 1:85:A:PRO:HB2 | 12 | 0.21 |
| (1,836) | 1:54:A:ARG:HG2 | 1:55:A:GLY:H | 17 | 0.21 |
| (1,817) | 1:107:A:LYS:HG2 | 1:107:A:LYS:HE3 | 19 | 0.21 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 11 | 0.21 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 3 | 0.21 |
| (1,810) | 1:107:A:LYS:HA | 1:107:A:LYS:HD3 | 10 | 0.21 |
| (1,804) | 1:105:A:GLN:HA | 1:105:A:GLN:HG2 | 20 | 0.21 |
| (1,785) | 1:92:A:ARG:H | 1:92:A:ARG:HG2 | 20 | 0.21 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 4 | 0.21 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 7 | 0.21 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 14 | 0.21 |
| (1,693) | 1:33:A:VAL:HA | 1:51:A:MET:HA | 1 | 0.21 |
| (1,684) | 1:121:A:LYS:HB2 | 1:122:A:ASP:H | 11 | 0.21 |
| (1,679) | 1:116:A:THR:HB | 1:117:A:GLY:H | 1 | 0.21 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 9 | 0.21 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 14 | 0.21 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 15 | 0.21 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 18 | 0.21 |
| (1,520) | 1:42:A:GLU:H | 1:42:A:GLU:HB3 | 5 | 0.21 |
| (1,520) | 1:42:A:GLU:H | 1:42:A:GLU:HB3 | 9 | 0.21 |
| (1,520) | 1:42:A:GLU:H | 1:42:A:GLU:HB3 | 10 | 0.21 |
| (1,520) | 1:42:A:GLU:H | 1:42:A:GLU:HB3 | 16 | 0.21 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 14 | 0.21 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 8 | 0.21 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 12 | 0.21 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 19 | 0.21 |
| (1,314) | 1:65:A:LYS:HG3 | 1:66:A:VAL:H | 17 | 0.21 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 5 | 0.21 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 7 | 0.21 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 13 | 0.21 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 4 | 0.21 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 3 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 3 | 0.2 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 8 | 0.2 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 8 | 0.2 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 16 | 0.2 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 16 | 0.2 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 17 | 0.2 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 17 | 0.2 |
| (1,1502) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 9 | 0.2 |
| (1,1502) | 1:65:A:LYS:H | 1:65:A:LYS:HG3 | 9 | 0.2 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 5 | 0.2 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 5 | 0.2 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 5 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 4 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 4 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 4 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 9 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 9 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 9 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 11 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 11 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 11 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 15 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 15 | 0.2 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 15 | 0.2 |
| (1,1281) | 1:99:A:ILE:HD11 | 1:109:A:MET:H | 18 | 0.2 |
| (1,1281) | 1:99:A:ILE:HD12 | 1:109:A:MET:H | 18 | 0.2 |
| (1,1281) | 1:99:A:ILE:HD13 | 1:109:A:MET:H | 18 | 0.2 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG21 | 5 | 0.2 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG22 | 5 | 0.2 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG23 | 5 | 0.2 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG21 | 10 | 0.2 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG22 | 10 | 0.2 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG23 | 10 | 0.2 |
| (1,922) | 1:89:A:THR:HB | 1:101:A:GLU:HG2 | 11 | 0.2 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 4 | 0.2 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 12 | 0.2 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 5 | 0.2 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 12 | 0.2 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 9 | 0.2 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 16 | 0.2 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 1 | 0.2 |
| (1,871) | 1:51:A:MET:HB2 | 1:54:A:ARG:HG3 | 17 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,846) | 1:78:A:GLN:HE21 | 1:85:A:PRO:HB2 | 9 | 0.2 |
| (1,837) | 1:54:A:ARG:HG3 | 1:55:A:GLY:H | 19 | 0.2 |
| (1,820) | 1:111:A:ARG:HA | 1:111:A:ARG:HG3 | 8 | 0.2 |
| (1,793) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HD3 | 6 | 0.2 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 20 | 0.2 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 3 | 0.2 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 10 | 0.2 |
| (1,737) | 1:34:A:LYS:H | 1:34:A:LYS:HG2 | 18 | 0.2 |
| (1,549) | 1:74:A:SER:H | 1:74:A:SER:HB2 | 9 | 0.2 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 14 | 0.2 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 16 | 0.2 |
| (1,3) | 1:13:A:GLU:HB2 | 1:14:A:THR:H | 12 | 0.2 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 7 | 0.19 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 7 | 0.19 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 11 | 0.19 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 11 | 0.19 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 14 | 0.19 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 14 | 0.19 |
| (1,1327) | 1:21:A:TRP:HA | 1:21:A:TRP:HE3 | 5 | 0.19 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 7 | 0.19 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 7 | 0.19 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 7 | 0.19 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 14 | 0.19 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 14 | 0.19 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 14 | 0.19 |
| (1,1281) | 1:99:A:ILE:HD11 | 1:109:A:MET:H | 14 | 0.19 |
| (1,1281) | 1:99:A:ILE:HD12 | 1:109:A:MET:H | 14 | 0.19 |
| (1,1281) | 1:99:A:ILE:HD13 | 1:109:A:MET:H | 14 | 0.19 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG21 | 9 | 0.19 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG22 | 9 | 0.19 |
| (1,1240) | 1:95:A:ASN:HB3 | 1:97:A:THR:HG23 | 9 | 0.19 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD11 | 13 | 0.19 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD12 | 13 | 0.19 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD13 | 13 | 0.19 |
| (1,1030) | 1:29:A:PRO:HB3 | 1:30:A:THR:HG21 | 8 | 0.19 |
| (1,1030) | 1:29:A:PRO:HB3 | 1:30:A:THR:HG22 | 8 | 0.19 |
| (1,1030) | 1:29:A:PRO:HB3 | 1:30:A:THR:HG23 | 8 | 0.19 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 20 | 0.19 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 3 | 0.19 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 7 | 0.19 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 10 | 0.19 |
| (1,906) | 1:88:A:SER:HB2 | 1:102:A:GLN:HG2 | 5 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 6 | 0.19 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 15 | 0.19 |
| (1,871) | 1:51:A:MET:HB2 | 1:54:A:ARG:HG3 | 7 | 0.19 |
| (1,851) | 1:111:A:ARG:HG3 | 1:112:A:ILE:H | 8 | 0.19 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 4 | 0.19 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 18 | 0.19 |
| (1,818) | 1:107:A:LYS:HG3 | 1:107:A:LYS:HE3 | 15 | 0.19 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 8 | 0.19 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 1 | 0.19 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 2 | 0.19 |
| (1,810) | 1:107:A:LYS:HA | 1:107:A:LYS:HD3 | 12 | 0.19 |
| (1,804) | 1:105:A:GLN:HA | 1:105:A:GLN:HG2 | 16 | 0.19 |
| (1,790) | 1:92:A:ARG:HB3 | 1:92:A:ARG:HD2 | 9 | 0.19 |
| (1,764) | 1:62:A:MET:HA | 1:62:A:MET:HG3 | 10 | 0.19 |
| (1,763) | 1:62:A:MET:H | 1:62:A:MET:HG3 | 11 | 0.19 |
| (1,751) | 1:56:A:GLU:H | 1:56:A:GLU:HG2 | 12 | 0.19 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 9 | 0.19 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 12 | 0.19 |
| (1,739) | 1:34:A:LYS:H | 1:34:A:LYS:HG3 | 10 | 0.19 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 13 | 0.19 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 6 | 0.19 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 17 | 0.19 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 3 | 0.19 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 9 | 0.19 |
| (1,520) | 1:42:A:GLU:H | 1:42:A:GLU:HB3 | 15 | 0.19 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 4 | 0.19 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 17 | 0.19 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 10 | 0.18 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 10 | 0.18 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 15 | 0.18 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 15 | 0.18 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 10 | 0.18 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 10 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 1 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 1 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 1 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 14 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 14 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 14 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 17 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 17 | 0.18 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 17 | 0.18 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 17 | 0.18 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 17 | 0.18 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD21 | 7 | 0.18 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD22 | 7 | 0.18 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD23 | 7 | 0.18 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 13 | 0.18 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 13 | 0.18 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 13 | 0.18 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 14 | 0.18 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 14 | 0.18 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 14 | 0.18 |
| (1,1055) | 1:38:A:VAL:HG21 | 1:100:A:TRP:HH2 | 7 | 0.18 |
| (1,1055) | 1:38:A:VAL:HG22 | 1:100:A:TRP:HH2 | 7 | 0.18 |
| (1,1055) | 1:38:A:VAL:HG23 | 1:100:A:TRP:HH2 | 7 | 0.18 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 9 | 0.18 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 10 | 0.18 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 14 | 0.18 |
| (1,909) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG2 | 20 | 0.18 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 6 | 0.18 |
| (1,908) | 1:88:A:SER:HB3 | 1:102:A:GLN:HG3 | 13 | 0.18 |
| (1,907) | 1:88:A:SER:HB2 | 1:102:A:GLN:HG3 | 7 | 0.18 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 12 | 0.18 |
| (1,882) | 1:68:A:SER:HB3 | 1:76:A:GLU:HB2 | 16 | 0.18 |
| (1,804) | 1:105:A:GLN:HA | 1:105:A:GLN:HG2 | 14 | 0.18 |
| (1,764) | 1:62:A:MET:HA | 1:62:A:MET:HG3 | 1 | 0.18 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 5 | 0.18 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 11 | 0.18 |
| (1,734) | 1:23:A:GLU:HA | 1:23:A:GLU:HG3 | 16 | 0.18 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 9 | 0.18 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 1 | 0.18 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 19 | 0.18 |
| (1,604) | 1:37:A:THR:HB | 1:38:A:VAL:H | 6 | 0.18 |
| (1,566) | 1:106:A:ARG:H | 1:106:A:ARG:HB2 | 2 | 0.18 |
| (1,566) | 1:106:A:ARG:H | 1:106:A:ARG:HB2 | 3 | 0.18 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 8 | 0.18 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 12 | 0.18 |
| (1,400) | 1:29:A:PRO:HG2 | 1:32:A:GLY:H | 5 | 0.18 |
| (1,400) | 1:29:A:PRO:HG3 | 1:32:A:GLY:H | 5 | 0.18 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 5 | 0.18 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 8 | 0.18 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 2 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,219) | 1:118:A:ARG:H | 1:119:A:GLU:H | 20 | 0.18 |
| (1,134) | 1:122:A:ASP:HB2 | 1:123:A:GLU:H | 8 | 0.18 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 13 | 0.17 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 13 | 0.17 |
| (1,1533) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG2 | 10 | 0.17 |
| (1,1533) | 1:74:A:SER:HB2 | 1:91:A:LYS:HG3 | 10 | 0.17 |
| (1,1533) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG2 | 10 | 0.17 |
| (1,1533) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG3 | 10 | 0.17 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 10 | 0.17 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 10 | 0.17 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 10 | 0.17 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD11 | 15 | 0.17 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD12 | 15 | 0.17 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD13 | 15 | 0.17 |
| (1,1126) | 1:65:A:LYS:HG3 | 1:80:A:LEU:HD21 | 9 | 0.17 |
| (1,1126) | 1:65:A:LYS:HG3 | 1:80:A:LEU:HD22 | 9 | 0.17 |
| (1,1126) | 1:65:A:LYS:HG3 | 1:80:A:LEU:HD23 | 9 | 0.17 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 11 | 0.17 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 11 | 0.17 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 11 | 0.17 |
| (1,1055) | 1:38:A:VAL:HG21 | 1:100:A:TRP:HH2 | 15 | 0.17 |
| (1,1055) | 1:38:A:VAL:HG22 | 1:100:A:TRP:HH2 | 15 | 0.17 |
| (1,1055) | 1:38:A:VAL:HG23 | 1:100:A:TRP:HH2 | 15 | 0.17 |
| (1,1040) | 1:36:A:ALA:HB1 | 1:49:A:GLU:HG3 | 20 | 0.17 |
| (1,1040) | 1:36:A:ALA:HB2 | 1:49:A:GLU:HG3 | 20 | 0.17 |
| (1,1040) | 1:36:A:ALA:HB3 | 1:49:A:GLU:HG3 | 20 | 0.17 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 16 | 0.17 |
| (1,884) | 1:68:A:SER:HB3 | 1:76:A:GLU:H | 15 | 0.17 |
| (1,849) | 1:105:A:GLN:HG2 | 1:106:A:ARG:H | 20 | 0.17 |
| (1,835) | 1:47:A:GLU:HG2 | 1:48:A:THR:H | 16 | 0.17 |
| (1,826) | 1:115:A:LYS:HA | 1:115:A:LYS:HG3 | 5 | 0.17 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 6 | 0.17 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 13 | 0.17 |
| (1,810) | 1:107:A:LYS:HA | 1:107:A:LYS:HD3 | 17 | 0.17 |
| (1,795) | 1:99:A:ILE:HA | 1:99:A:ILE:HG12 | 4 | 0.17 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 13 | 0.17 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 14 | 0.17 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 6 | 0.17 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 8 | 0.17 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 13 | 0.17 |
| (1,737) | 1:34:A:LYS:H | 1:34:A:LYS:HG2 | 2 | 0.17 |
| (1,737) | 1:34:A:LYS:H | 1:34:A:LYS:HG2 | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,737) | 1:34:A:LYS:H | 1:34:A:LYS:HG2 | 19 | 0.17 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 10 | 0.17 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 12 | 0.17 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 13 | 0.17 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 5 | 0.17 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 5 | 0.17 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 7 | 0.17 |
| (1,531) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 19 | 0.17 |
| (1,400) | 1:29:A:PRO:HG2 | 1:32:A:GLY:H | 20 | 0.17 |
| (1,400) | 1:29:A:PRO:HG3 | 1:32:A:GLY:H | 20 | 0.17 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 9 | 0.17 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 5 | 0.17 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 11 | 0.17 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 20 | 0.17 |
| (1,219) | 1:118:A:ARG:H | 1:119:A:GLU:H | 3 | 0.17 |
| (1,181) | 1:118:A:ARG:H | 1:118:A:ARG:HB2 | 10 | 0.17 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 4 | 0.16 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 4 | 0.16 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 20 | 0.16 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 20 | 0.16 |
| (1,1359) | 1:17:A:TYR:HA | 1:21:A:TRP:HZ2 | 12 | 0.16 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 15 | 0.16 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 15 | 0.16 |
| (1,1325) | 1:17:A:TYR:HE1 | 1:75:A:ILE:HG12 | 13 | 0.16 |
| (1,1325) | 1:17:A:TYR:HE2 | 1:75:A:ILE:HG12 | 13 | 0.16 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD11 | 8 | 0.16 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD12 | 8 | 0.16 |
| (1,1268) | 1:91:A:LYS:HB3 | 1:99:A:ILE:HD13 | 8 | 0.16 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG21 | 4 | 0.16 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG22 | 4 | 0.16 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG23 | 4 | 0.16 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD21 | 16 | 0.16 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD22 | 16 | 0.16 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD23 | 16 | 0.16 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 4 | 0.16 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 4 | 0.16 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 4 | 0.16 |
| (1,1055) | 1:38:A:VAL:HG21 | 1:100:A:TRP:HH2 | 11 | 0.16 |
| (1,1055) | 1:38:A:VAL:HG22 | 1:100:A:TRP:HH2 | 11 | 0.16 |
| (1,1055) | 1:38:A:VAL:HG23 | 1:100:A:TRP:HH2 | 11 | 0.16 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 11 | 0.16 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 14 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 19 | 0.16 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 11 | 0.16 |
| (1,764) | 1:62:A:MET:HA | 1:62:A:MET:HG3 | 11 | 0.16 |
| (1,764) | 1:62:A:MET:HA | 1:62:A:MET:HG3 | 19 | 0.16 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 20 | 0.16 |
| (1,713) | 1:80:A:LEU:HA | 1:84:A:TYR:HB3 | 19 | 0.16 |
| (1,531) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 10 | 0.16 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 9 | 0.16 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 3 | 0.16 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 9 | 0.16 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 15 | 0.16 |
| (1,337) | 1:107:A:LYS:HG3 | 1:108:A:THR:H | 20 | 0.16 |
| (1,314) | 1:65:A:LYS:HG3 | 1:66:A:VAL:H | 8 | 0.16 |
| (1,304) | 1:71:A:THR:HA | 1:73:A:GLY:H | 12 | 0.16 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 8 | 0.16 |
| (1,1359) | 1:17:A:TYR:HA | 1:21:A:TRP:HZ2 | 8 | 0.15 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 7 | 0.15 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 7 | 0.15 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 7 | 0.15 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD11 | 5 | 0.15 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD12 | 5 | 0.15 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD13 | 5 | 0.15 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD21 | 9 | 0.15 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD22 | 9 | 0.15 |
| (1,1125) | 1:65:A:LYS:HG2 | 1:80:A:LEU:HD23 | 9 | 0.15 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 8 | 0.15 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 8 | 0.15 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 8 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 7 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 7 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 7 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 9 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 9 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 9 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 10 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 10 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 10 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 20 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 20 | 0.15 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 20 | 0.15 |
| (1,938) | 1:75:A:ILE:H | 1:75:A:ILE:HG12 | 18 | 0.15 |
| (1,913) | 1:89:A:THR:HB | 1:101:A:GLU:HB2 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HG3 | 15 | 0.15 |
| (1,826) | 1:115:A:LYS:HA | 1:115:A:LYS:HG3 | 11 | 0.15 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 1 | 0.15 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 5 | 0.15 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 10 | 0.15 |
| (1,820) | 1:111:A:ARG:HA | 1:111:A:ARG:HG3 | 12 | 0.15 |
| (1,814) | 1:107:A:LYS:HG3 | 1:107:A:LYS:HE2 | 10 | 0.15 |
| (1,795) | 1:99:A:ILE:HA | 1:99:A:ILE:HG12 | 8 | 0.15 |
| (1,764) | 1:62:A:MET:HA | 1:62:A:MET:HG3 | 13 | 0.15 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 2 | 0.15 |
| (1,737) | 1:34:A:LYS:H | 1:34:A:LYS:HG2 | 14 | 0.15 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 15 | 0.15 |
| (1,641) | 1:74:A:SER:HB3 | 1:75:A:ILE:H | 18 | 0.15 |
| (1,640) | 1:74:A:SER:HB2 | 1:75:A:ILE:H | 1 | 0.15 |
| (1,637) | 1:71:A:THR:HB | 1:72:A:ASP:H | 3 | 0.15 |
| (1,624) | 1:54:A:ARG:HB2 | 1:55:A:GLY:H | 6 | 0.15 |
| (1,569) | 1:110:A:THR:H | 1:110:A:THR:HB | 10 | 0.15 |
| (1,566) | 1:106:A:ARG:H | 1:106:A:ARG:HB2 | 16 | 0.15 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 8 | 0.15 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 11 | 0.15 |
| (1,534) | 1:54:A:ARG:H | 1:54:A:ARG:HB3 | 17 | 0.15 |
| (1,531) | 1:52:A:GLU:H | 1:52:A:GLU:HB2 | 7 | 0.15 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 1 | 0.15 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 18 | 0.15 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 4 | 0.14 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 4 | 0.14 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 14 | 0.14 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 14 | 0.14 |
| (1,1548) | 1:78:A:GLN:HG2 | 1:80:A:LEU:HG | 9 | 0.14 |
| (1,1548) | 1:78:A:GLN:HG3 | 1:80:A:LEU:HG | 9 | 0.14 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 14 | 0.14 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 14 | 0.14 |
| (1,1325) | 1:17:A:TYR:HE1 | 1:75:A:ILE:HG12 | 1 | 0.14 |
| (1,1325) | 1:17:A:TYR:HE2 | 1:75:A:ILE:HG12 | 1 | 0.14 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 9 | 0.14 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 9 | 0.14 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 9 | 0.14 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD11 | 10 | 0.14 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD12 | 10 | 0.14 |
| (1,1290) | 1:38:A:VAL:H | 1:112:A:ILE:HD13 | 10 | 0.14 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG21 | 13 | 0.14 |
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG22 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1287) | 1:97:A:THR:HA | 1:110:A:THR:HG23 | 13 | 0.14 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG21 | 20 | 0.14 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG22 | 20 | 0.14 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG23 | 20 | 0.14 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 9 | 0.14 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 9 | 0.14 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 9 | 0.14 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 2 | 0.14 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 2 | 0.14 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 2 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB1 | 1:49:A:GLU:HG3 | 2 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB2 | 1:49:A:GLU:HG3 | 2 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB3 | 1:49:A:GLU:HG3 | 2 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB1 | 1:49:A:GLU:HG3 | 7 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB2 | 1:49:A:GLU:HG3 | 7 | 0.14 |
| (1,1040) | 1:36:A:ALA:HB3 | 1:49:A:GLU:HG3 | 7 | 0.14 |
| (1,938) | 1:75:A:ILE:H | 1:75:A:ILE:HG12 | 19 | 0.14 |
| (1,886) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG3 | 1 | 0.14 |
| (1,871) | 1:51:A:MET:HB2 | 1:54:A:ARG:HG3 | 18 | 0.14 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 19 | 0.14 |
| (1,820) | 1:111:A:ARG:HA | 1:111:A:ARG:HG3 | 9 | 0.14 |
| (1,818) | 1:107:A:LYS:HG3 | 1:107:A:LYS:HE3 | 16 | 0.14 |
| (1,795) | 1:99:A:ILE:HA | 1:99:A:ILE:HG12 | 17 | 0.14 |
| (1,734) | 1:23:A:GLU:HA | 1:23:A:GLU:HG3 | 13 | 0.14 |
| (1,684) | 1:121:A:LYS:HB2 | 1:122:A:ASP:H | 5 | 0.14 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 11 | 0.14 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 12 | 0.14 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 18 | 0.14 |
| (1,640) | 1:74:A:SER:HB2 | 1:75:A:ILE:H | 12 | 0.14 |
| (1,582) | 1:8:A:GLN:HA | 1:9:A:GLN:H | 10 | 0.14 |
| (1,550) | 1:74:A:SER:H | 1:74:A:SER:HB3 | 7 | 0.14 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 19 | 0.14 |
| (1,413) | 1:78:A:GLN:HE21 | 1:85:A:PRO:HB3 | 1 | 0.14 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 17 | 0.14 |
| (1,354) | 1:54:A:ARG:H | 1:54:A:ARG:HG3 | 17 | 0.14 |
| (1,354) | 1:54:A:ARG:H | 1:54:A:ARG:HG3 | 18 | 0.14 |
| (1,314) | 1:65:A:LYS:HG3 | 1:66:A:VAL:H | 1 | 0.14 |
| (1,310) | 1:47:A:GLU:HG3 | 1:48:A:THR:H | 11 | 0.14 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 1 | 0.14 |
| (1,275) | 1:84:A:TYR:H | 1:85:A:PRO:HA | 18 | 0.14 |
| (1,1325) | 1:17:A:TYR:HE1 | 1:75:A:ILE:HG12 | 5 | 0.13 |
| (1,1325) | 1:17:A:TYR:HE2 | 1:75:A:ILE:HG12 | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1325) | 1:17:A:TYR:HE1 | 1:75:A:ILE:HG12 | 12 | 0.13 |
| (1,1325) | 1:17:A:TYR:HE2 | 1:75:A:ILE:HG12 | 12 | 0.13 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG21 | 13 | 0.13 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG22 | 13 | 0.13 |
| (1,1321) | 1:99:A:ILE:HA | 1:108:A:THR:HG23 | 13 | 0.13 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 6 | 0.13 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 6 | 0.13 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 6 | 0.13 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD11 | 16 | 0.13 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD12 | 16 | 0.13 |
| (1,1156) | 1:69:A:GLN:HB3 | 1:75:A:ILE:HD13 | 16 | 0.13 |
| (1,1094) | 1:46:A:VAL:HG21 | 1:59:A:LEU:H | 4 | 0.13 |
| (1,1094) | 1:46:A:VAL:HG22 | 1:59:A:LEU:H | 4 | 0.13 |
| (1,1094) | 1:46:A:VAL:HG23 | 1:59:A:LEU:H | 4 | 0.13 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 10 | 0.13 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 10 | 0.13 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 10 | 0.13 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB1 | 13 | 0.13 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB2 | 13 | 0.13 |
| (1,1043) | 1:23:A:GLU:HB3 | 1:36:A:ALA:HB3 | 13 | 0.13 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG21 | 20 | 0.13 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG22 | 20 | 0.13 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG23 | 20 | 0.13 |
| (1,931) | 1:22:A:ASP:HB2 | 1:112:A:ILE:HG12 | 8 | 0.13 |
| (1,896) | 1:67:A:ILE:HG12 | 1:77:A:ILE:HA | 4 | 0.13 |
| (1,849) | 1:105:A:GLN:HG2 | 1:106:A:ARG:H | 2 | 0.13 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 7 | 0.13 |
| (1,817) | 1:107:A:LYS:HG2 | 1:107:A:LYS:HE3 | 1 | 0.13 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 14 | 0.13 |
| (1,815) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 16 | 0.13 |
| (1,814) | 1:107:A:LYS:HG3 | 1:107:A:LYS:HE2 | 5 | 0.13 |
| (1,813) | 1:107:A:LYS:HG2 | 1:107:A:LYS:HE2 | 7 | 0.13 |
| (1,795) | 1:99:A:ILE:HA | 1:99:A:ILE:HG12 | 6 | 0.13 |
| (1,795) | 1:99:A:ILE:HA | 1:99:A:ILE:HG12 | 19 | 0.13 |
| (1,763) | 1:62:A:MET:H | 1:62:A:MET:HG3 | 19 | 0.13 |
| (1,751) | 1:56:A:GLU:H | 1:56:A:GLU:HG2 | 14 | 0.13 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 2 | 0.13 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 18 | 0.13 |
| (1,737) | 1:34:A:LYS:H | 1:34:A:LYS:HG2 | 20 | 0.13 |
| (1,724) | 1:29:A:PRO:HB3 | 1:31:A:ASP:H | 3 | 0.13 |
| (1,678) | 1:116:A:THR:HA | 1:117:A:GLY:H | 4 | 0.13 |
| (1,669) | 1:103:A:ASN:HA | 1:104:A:GLY:H | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 18 | 0.13 |
| (1,566) | 1:106:A:ARG:H | 1:106:A:ARG:HB2 | 13 | 0.13 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 15 | 0.13 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 17 | 0.13 |
| (1,532) | 1:52:A:GLU:H | 1:52:A:GLU:HB3 | 17 | 0.13 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 3 | 0.13 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 18 | 0.13 |
| (1,415) | 1:78:A:GLN:HE22 | 1:85:A:PRO:HB2 | 20 | 0.13 |
| (1,413) | 1:78:A:GLN:HE21 | 1:85:A:PRO:HB3 | 18 | 0.13 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 19 | 0.13 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 20 | 0.13 |
| (1,314) | 1:65:A:LYS:HG3 | 1:66:A:VAL:H | 13 | 0.13 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 10 | 0.13 |
| (1,185) | 1:123:A:GLU:H | 1:123:A:GLU:HB3 | 8 | 0.13 |
| (1,143) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 17 | 0.13 |
| (1,1357) | 1:84:A:TYR:HE1 | 1:85:A:PRO:HA | 2 | 0.12 |
| (1,1357) | 1:84:A:TYR:HE2 | 1:85:A:PRO:HA | 2 | 0.12 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 15 | 0.12 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 15 | 0.12 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 15 | 0.12 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG21 | 5 | 0.12 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG22 | 5 | 0.12 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG23 | 5 | 0.12 |
| (1,1205) | 1:86:A:LEU:HD11 | 1:103:A:ASN:HD22 | 13 | 0.12 |
| (1,1205) | 1:86:A:LEU:HD12 | 1:103:A:ASN:HD22 | 13 | 0.12 |
| (1,1205) | 1:86:A:LEU:HD13 | 1:103:A:ASN:HD22 | 13 | 0.12 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 14 | 0.12 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 14 | 0.12 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 14 | 0.12 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 6 | 0.12 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 6 | 0.12 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 6 | 0.12 |
| (1,1073) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HH2 | 16 | 0.12 |
| (1,1073) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HH2 | 16 | 0.12 |
| (1,1073) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HH2 | 16 | 0.12 |
| (1,1070) | 1:45:A:VAL:HG11 | 1:100:A:TRP:HZ2 | 11 | 0.12 |
| (1,1070) | 1:45:A:VAL:HG12 | 1:100:A:TRP:HZ2 | 11 | 0.12 |
| (1,1070) | 1:45:A:VAL:HG13 | 1:100:A:TRP:HZ2 | 11 | 0.12 |
| (1,1040) | 1:36:A:ALA:HB1 | 1:49:A:GLU:HG3 | 15 | 0.12 |
| (1,1040) | 1:36:A:ALA:HB2 | 1:49:A:GLU:HG3 | 15 | 0.12 |
| (1,1040) | 1:36:A:ALA:HB3 | 1:49:A:GLU:HG3 | 15 | 0.12 |
| (1,912) | 1:89:A:THR:HB | 1:101:A:GLU:HB3 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,904) | 1:88:A:SER:HB3 | 1:102:A:GLN:HA | 14 | 0.12 |
| (1,886) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG3 | 14 | 0.12 |
| (1,861) | 1:65:A:LYS:HG2 | 1:66:A:VAL:H | 18 | 0.12 |
| (1,826) | 1:115:A:LYS:HA | 1:115:A:LYS:HG3 | 13 | 0.12 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 8 | 0.12 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 15 | 0.12 |
| (1,761) | 1:62:A:MET:H | 1:62:A:MET:HG2 | 18 | 0.12 |
| (1,747) | 1:54:A:ARG:HA | 1:54:A:ARG:HG3 | 1 | 0.12 |
| (1,706) | 1:70:A:SER:HB2 | 1:73:A:GLY:H | 15 | 0.12 |
| (1,706) | 1:70:A:SER:HB2 | 1:73:A:GLY:H | 19 | 0.12 |
| (1,674) | 1:110:A:THR:HB | 1:111:A:ARG:H | 3 | 0.12 |
| (1,674) | 1:110:A:THR:HB | 1:111:A:ARG:H | 6 | 0.12 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 17 | 0.12 |
| (1,641) | 1:74:A:SER:HB3 | 1:75:A:ILE:H | 19 | 0.12 |
| (1,640) | 1:74:A:SER:HB2 | 1:75:A:ILE:H | 17 | 0.12 |
| (1,625) | 1:54:A:ARG:HB3 | 1:55:A:GLY:H | 6 | 0.12 |
| (1,550) | 1:74:A:SER:H | 1:74:A:SER:HB3 | 4 | 0.12 |
| (1,546) | 1:71:A:THR:HA | 1:71:A:THR:HB | 6 | 0.12 |
| (1,546) | 1:71:A:THR:HA | 1:71:A:THR:HB | 10 | 0.12 |
| (1,546) | 1:71:A:THR:HA | 1:71:A:THR:HB | 19 | 0.12 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 3 | 0.12 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 5 | 0.12 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 9 | 0.12 |
| (1,429) | 1:102:A:GLN:HG3 | 1:103:A:ASN:HD21 | 3 | 0.12 |
| (1,429) | 1:102:A:GLN:HG3 | 1:103:A:ASN:HD21 | 18 | 0.12 |
| (1,415) | 1:78:A:GLN:HE22 | 1:85:A:PRO:HB2 | 13 | 0.12 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 11 | 0.12 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 16 | 0.12 |
| (1,367) | 1:91:A:LYS:H | 1:91:A:LYS:HG3 | 3 | 0.12 |
| (1,354) | 1:54:A:ARG:H | 1:54:A:ARG:HG3 | 8 | 0.12 |
| (1,326) | 1:91:A:LYS:HG3 | 1:92:A:ARG:H | 6 | 0.12 |
| (1,314) | 1:65:A:LYS:HG3 | 1:66:A:VAL:H | 16 | 0.12 |
| (1,305) | 1:65:A:LYS:H | 1:80:A:LEU:H | 7 | 0.12 |
| (1,198) | 1:49:A:GLU:H | 1:59:A:LEU:H | 14 | 0.12 |
| (1,1358) | 1:88:A:SER:HG | 1:100:A:TRP:HD1 | 13 | 0.11 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD11 | 18 | 0.11 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD12 | 18 | 0.11 |
| (1,1300) | 1:37:A:THR:HB | 1:112:A:ILE:HD13 | 18 | 0.11 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG21 | 18 | 0.11 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG22 | 18 | 0.11 |
| (1,1210) | 1:76:A:GLU:HG2 | 1:89:A:THR:HG23 | 18 | 0.11 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG21 | 19 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG22 | 19 | 0.11 |
| (1,1029) | 1:29:A:PRO:HB2 | 1:30:A:THR:HG23 | 19 | 0.11 |
| (1,940) | 1:74:A:SER:HB3 | 1:91:A:LYS:HG2 | 10 | 0.11 |
| (1,913) | 1:89:A:THR:HB | 1:101:A:GLU:HB2 | 19 | 0.11 |
| (1,824) | 1:112:A:ILE:H | 1:112:A:ILE:HG13 | 17 | 0.11 |
| (1,817) | 1:107:A:LYS:HG2 | 1:107:A:LYS:HE3 | 14 | 0.11 |
| (1,765) | 1:65:A:LYS:H | 1:65:A:LYS:HG2 | 8 | 0.11 |
| (1,751) | 1:56:A:GLU:H | 1:56:A:GLU:HG2 | 10 | 0.11 |
| (1,751) | 1:56:A:GLU:H | 1:56:A:GLU:HG2 | 18 | 0.11 |
| (1,728) | 1:43:A:ASP:HA | 1:64:A:TYR:H | 1 | 0.11 |
| (1,706) | 1:70:A:SER:HB2 | 1:73:A:GLY:H | 4 | 0.11 |
| (1,674) | 1:110:A:THR:HB | 1:111:A:ARG:H | 7 | 0.11 |
| (1,669) | 1:103:A:ASN:HA | 1:104:A:GLY:H | 11 | 0.11 |
| (1,660) | 1:94:A:GLU:HA | 1:95:A:ASN:H | 8 | 0.11 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 6 | 0.11 |
| (1,644) | 1:76:A:GLU:HB3 | 1:77:A:ILE:H | 13 | 0.11 |
| (1,640) | 1:74:A:SER:HB2 | 1:75:A:ILE:H | 2 | 0.11 |
| (1,640) | 1:74:A:SER:HB2 | 1:75:A:ILE:H | 14 | 0.11 |
| (1,625) | 1:54:A:ARG:HB3 | 1:55:A:GLY:H | 2 | 0.11 |
| (1,622) | 1:51:A:MET:HB2 | 1:52:A:GLU:H | 16 | 0.11 |
| (1,592) | 1:29:A:PRO:HA | 1:30:A:THR:H | 8 | 0.11 |
| (1,567) | 1:106:A:ARG:H | 1:106:A:ARG:HB3 | 8 | 0.11 |
| (1,546) | 1:71:A:THR:HA | 1:71:A:THR:HB | 4 | 0.11 |
| (1,546) | 1:71:A:THR:HA | 1:71:A:THR:HB | 8 | 0.11 |
| (1,546) | 1:71:A:THR:HA | 1:71:A:THR:HB | 9 | 0.11 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 7 | 0.11 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 9 | 0.11 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 13 | 0.11 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 19 | 0.11 |
| (1,527) | 1:48:A:THR:H | 1:48:A:THR:HB | 8 | 0.11 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 8 | 0.11 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 11 | 0.11 |
| (1,425) | 1:94:A:GLU:HB3 | 1:95:A:ASN:HD22 | 10 | 0.11 |
| (1,415) | 1:78:A:GLN:HE22 | 1:85:A:PRO:HB2 | 19 | 0.11 |
| (1,398) | 1:22:A:ASP:H | 1:112:A:ILE:HG13 | 6 | 0.11 |
| (1,354) | 1:54:A:ARG:H | 1:54:A:ARG:HG3 | 15 | 0.11 |
| (1,314) | 1:65:A:LYS:HG3 | 1:66:A:VAL:H | 20 | 0.11 |
| (1,312) | 1:56:A:GLU:HG2 | 1:57:A:VAL:H | 20 | 0.11 |
| (1,309) | 1:44:A:GLU:HG3 | 1:45:A:VAL:H | 10 | 0.11 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 19 | 0.1 |
| (1,1634) | 1:107:A:LYS:HA | 1:107:A:LYS:HE3 | 19 | 0.1 |
| (1,1362) | 1:17:A:TYR:HE1 | 1:75:A:ILE:HG13 | 9 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1362) | 1:17:A:TYR:HE2 | 1:75:A:ILE:HG13 | 9 | 0.1 |
| (1,1327) | 1:21:A:TRP:HA | 1:21:A:TRP:HE3 | 10 | 0.1 |
| (1,1297) | 1:22:A:ASP:HB2 | 1:112:A:ILE:HD11 | 1 | 0.1 |
| (1,1297) | 1:22:A:ASP:HB2 | 1:112:A:ILE:HD12 | 1 | 0.1 |
| (1,1297) | 1:22:A:ASP:HB2 | 1:112:A:ILE:HD13 | 1 | 0.1 |
| (1,1084) | 1:46:A:VAL:HG11 | 1:58:A:GLN:HG3 | 7 | 0.1 |
| (1,1084) | 1:46:A:VAL:HG12 | 1:58:A:GLN:HG3 | 7 | 0.1 |
| (1,1084) | 1:46:A:VAL:HG13 | 1:58:A:GLN:HG3 | 7 | 0.1 |
| (1,1040) | 1:36:A:ALA:HB1 | 1:49:A:GLU:HG3 | 10 | 0.1 |
| (1,1040) | 1:36:A:ALA:HB2 | 1:49:A:GLU:HG3 | 10 | 0.1 |
| (1,1040) | 1:36:A:ALA:HB3 | 1:49:A:GLU:HG3 | 10 | 0.1 |
| (1,861) | 1:65:A:LYS:HG2 | 1:66:A:VAL:H | 14 | 0.1 |
| (1,826) | 1:115:A:LYS:HA | 1:115:A:LYS:HG3 | 17 | 0.1 |
| (1,818) | 1:107:A:LYS:HG3 | 1:107:A:LYS:HE3 | 20 | 0.1 |
| (1,817) | 1:107:A:LYS:HG2 | 1:107:A:LYS:HE3 | 2 | 0.1 |
| (1,817) | 1:107:A:LYS:HG2 | 1:107:A:LYS:HE3 | 13 | 0.1 |
| (1,811) | 1:107:A:LYS:HA | 1:107:A:LYS:HE2 | 9 | 0.1 |
| (1,751) | 1:56:A:GLU:H | 1:56:A:GLU:HG2 | 20 | 0.1 |
| (1,712) | 1:80:A:LEU:HA | 1:84:A:TYR:HB2 | 7 | 0.1 |
| (1,710) | 1:69:A:GLN:HA | 1:70:A:SER:HB3 | 10 | 0.1 |
| (1,706) | 1:70:A:SER:HB2 | 1:73:A:GLY:H | 11 | 0.1 |
| (1,640) | 1:74:A:SER:HB2 | 1:75:A:ILE:H | 5 | 0.1 |
| (1,567) | 1:106:A:ARG:H | 1:106:A:ARG:HB3 | 10 | 0.1 |
| (1,550) | 1:74:A:SER:H | 1:74:A:SER:HB3 | 5 | 0.1 |
| (1,550) | 1:74:A:SER:H | 1:74:A:SER:HB3 | 15 | 0.1 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 1 | 0.1 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 10 | 0.1 |
| (1,536) | 1:56:A:GLU:H | 1:56:A:GLU:HB3 | 12 | 0.1 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 2 | 0.1 |
| (1,516) | 1:34:A:LYS:H | 1:34:A:LYS:HB3 | 20 | 0.1 |
| (1,413) | 1:78:A:GLN:HE21 | 1:85:A:PRO:HB3 | 5 | 0.1 |
| (1,370) | 1:99:A:ILE:H | 1:99:A:ILE:HG13 | 4 | 0.1 |
| (1,345) | 1:23:A:GLU:H | 1:23:A:GLU:HG3 | 3 | 0.1 |

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

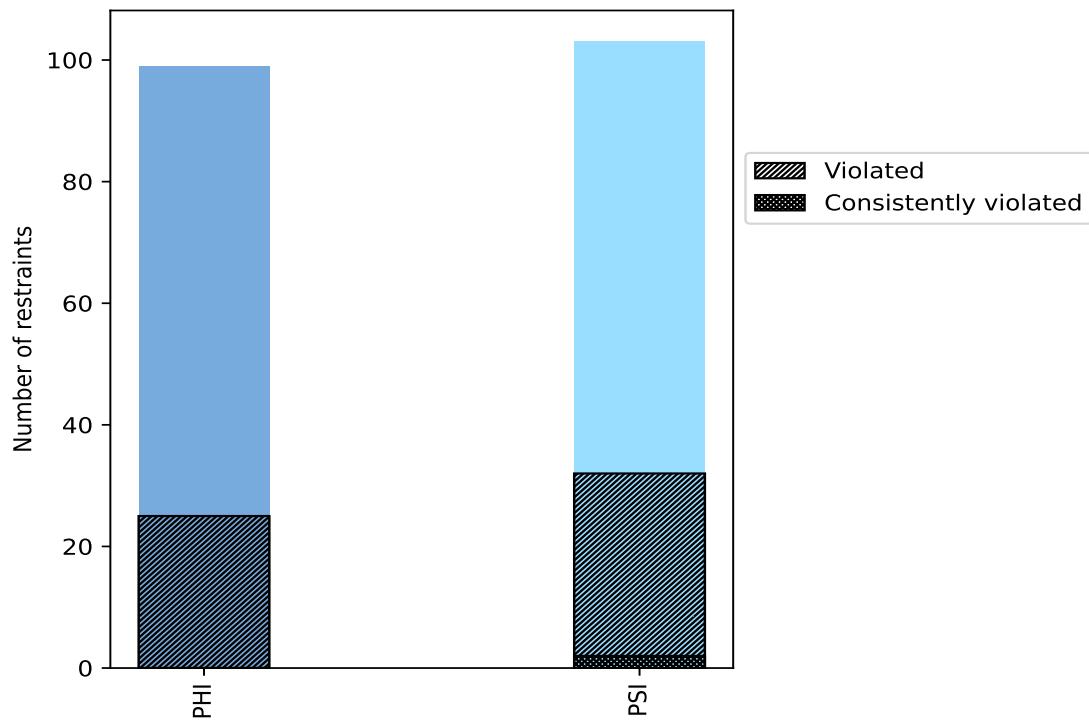
10.1 Summary of dihedral-angle violations [\(i\)](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PHI | 99 | 49.0 | 25 | 25.3 | 12.4 | 0 | 0.0 | 0.0 |
| PSI | 103 | 51.0 | 32 | 31.1 | 15.8 | 2 | 1.9 | 1.0 |
| Total | 202 | 100.0 | 57 | 28.2 | 28.2 | 2 | 1.0 | 1.0 |

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 [\(i\)](#)



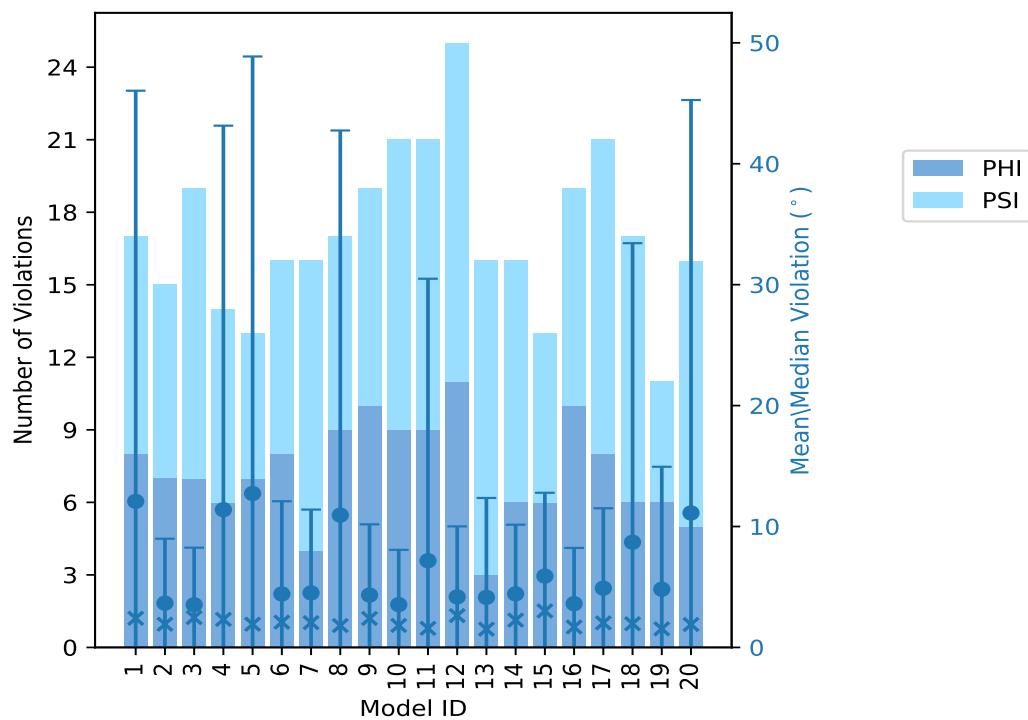
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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 (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PHI | PSI | Total | | | | |
| 1 | 8 | 9 | 17 | 12.08 | 146.65 | 33.96 | 2.41 |
| 2 | 7 | 8 | 15 | 3.66 | 23.17 | 5.33 | 1.92 |
| 3 | 7 | 12 | 19 | 3.53 | 23.07 | 4.72 | 2.47 |
| 4 | 6 | 8 | 14 | 11.39 | 125.81 | 31.76 | 2.32 |
| 5 | 7 | 6 | 13 | 12.73 | 137.78 | 36.14 | 1.92 |
| 6 | 8 | 8 | 16 | 4.42 | 33.69 | 7.67 | 2.09 |
| 7 | 4 | 12 | 16 | 4.51 | 29.71 | 6.89 | 2.05 |
| 8 | 9 | 8 | 17 | 10.94 | 137.45 | 31.81 | 1.81 |
| 9 | 10 | 9 | 19 | 4.33 | 27.22 | 5.85 | 2.4 |
| 10 | 9 | 12 | 21 | 3.54 | 22.63 | 4.53 | 1.82 |
| 11 | 9 | 12 | 21 | 7.17 | 111.24 | 23.32 | 1.58 |
| 12 | 11 | 14 | 25 | 4.18 | 31.07 | 5.83 | 2.63 |
| 13 | 3 | 13 | 16 | 4.14 | 35.7 | 8.22 | 1.51 |
| 14 | 6 | 10 | 16 | 4.43 | 25.27 | 5.72 | 2.26 |
| 15 | 6 | 7 | 13 | 5.9 | 23.81 | 6.89 | 3.02 |
| 16 | 10 | 9 | 19 | 3.62 | 19.51 | 4.61 | 1.69 |
| 17 | 8 | 13 | 21 | 4.9 | 26.48 | 6.61 | 2.03 |
| 18 | 6 | 11 | 17 | 8.7 | 107.46 | 24.73 | 1.96 |
| 19 | 6 | 5 | 11 | 4.81 | 36.81 | 10.13 | 1.54 |
| 20 | 5 | 11 | 16 | 11.12 | 143.26 | 34.15 | 1.9 |

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.

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

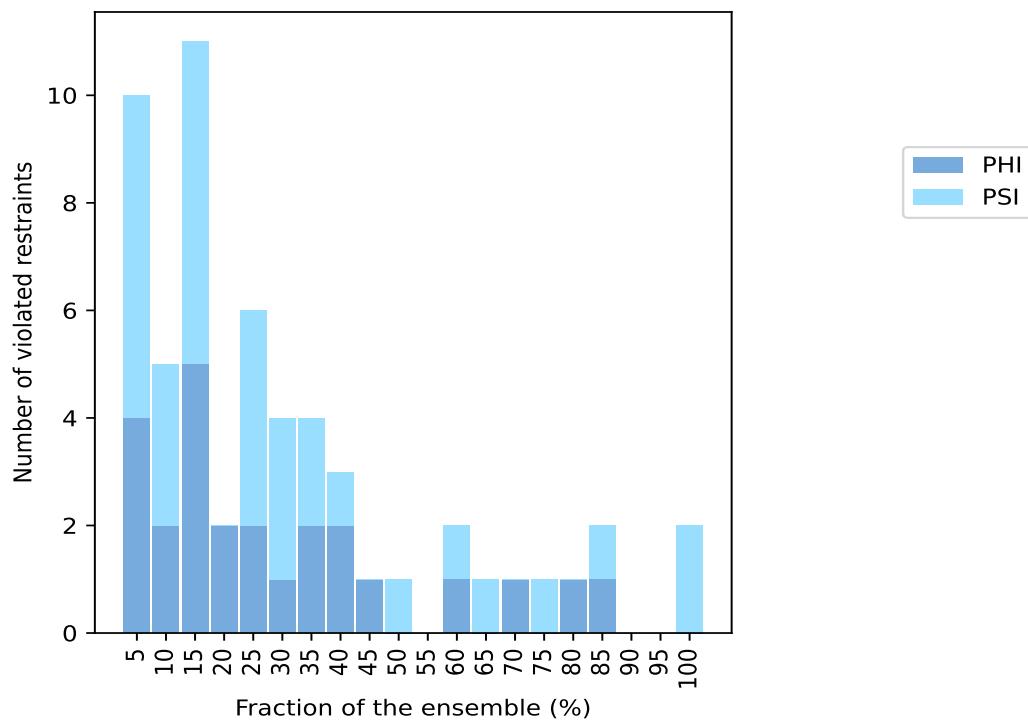
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI | PSI | Total | Count ¹ | % |
| 1 | 1 | 2 | 12 | 60.0 |
| 0 | 1 | 1 | 13 | 65.0 |
| 1 | 0 |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

¹ Number of models with violations

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

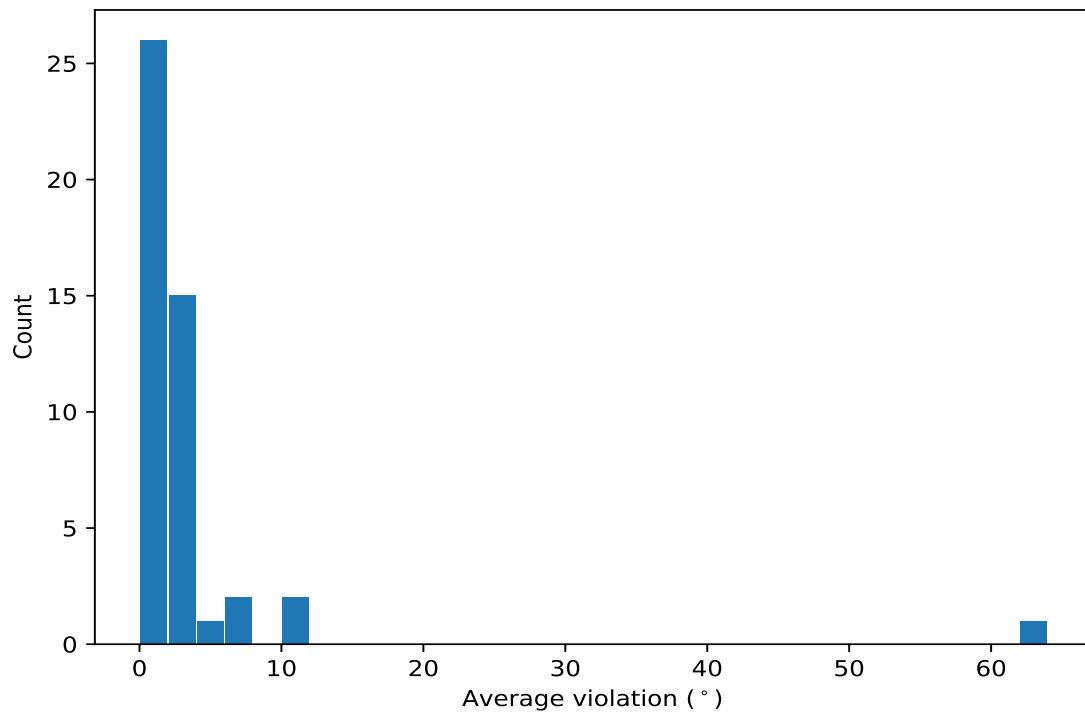


10.4 Most violated dihedral-angle restraints in the ensemble [\(i\)](#)

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

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

in the ensemble



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 20 | 63.39 | 49.76 | 32.38 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 20 | 3.35 | 1.69 | 3.07 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 17 | 3.4 | 1.29 | 4.1 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 17 | 1.89 | 0.49 | 1.75 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 16 | 2.88 | 1.07 | 2.76 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 15 | 7.08 | 6.03 | 5.01 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 14 | 2.06 | 0.49 | 2.12 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 13 | 1.72 | 0.52 | 1.52 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 12 | 2.73 | 0.85 | 2.57 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 12 | 1.85 | 0.74 | 1.85 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 10 | 2.44 | 0.84 | 2.18 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 9 | 4.18 | 2.08 | 3.5 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 8 | 2.51 | 0.8 | 2.78 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 8 | 2.01 | 0.89 | 1.62 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 8 | 1.43 | 0.35 | 1.26 |
| (1,89) | 1:16:A:PHE:C | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 7 | 3.86 | 1.94 | 3.2 |
| (1,84) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:MET:N | 7 | 1.99 | 0.81 | 1.8 |
| (1,34) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLN:N | 7 | 1.67 | 0.43 | 1.71 |
| (1,9) | 1:36:A:ALA:C | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 7 | 1.39 | 0.38 | 1.13 |
| (1,17) | 1:40:A:PHE:C | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 6 | 1.97 | 0.81 | 1.7 |

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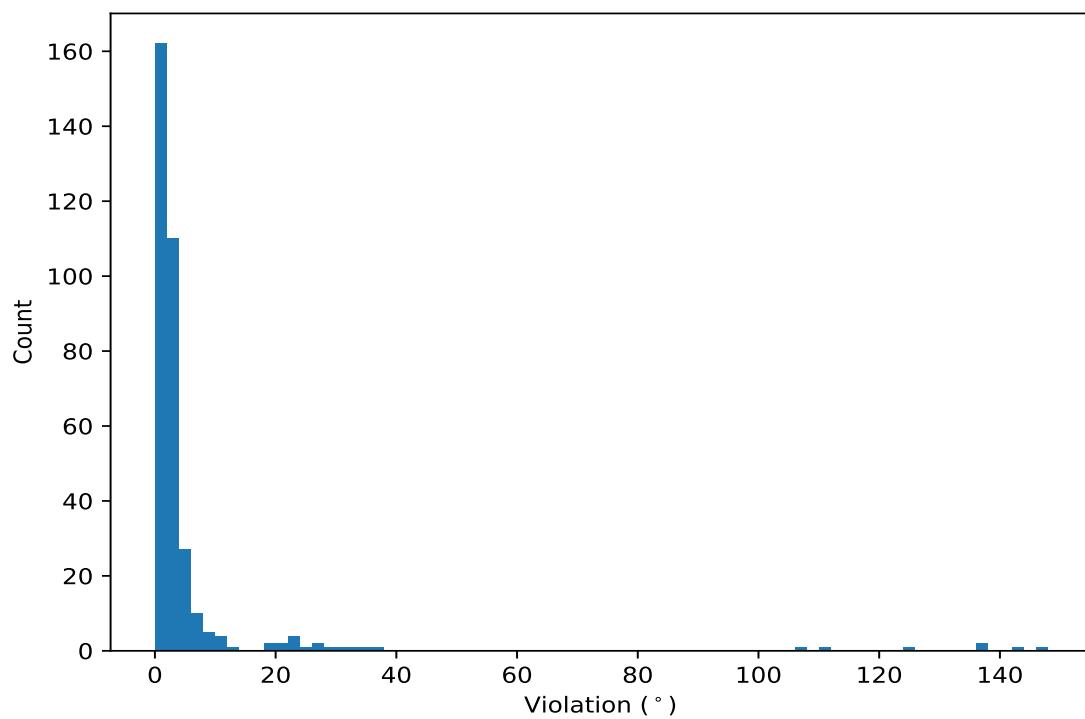
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,116) | 1:28:A:GLY:N | 1:28:A:GLY:CA | 1:28:A:GLY:C | 1:29:A:PRO:N | 6 | 1.84 | 0.87 | 1.54 |
| (1,66) | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 1:98:A:LEU:N | 6 | 1.77 | 0.57 | 1.74 |
| (1,80) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 1:107:A:LYS:N | 6 | 1.73 | 0.62 | 1.47 |
| (1,186) | 1:111:A:ARG:C | 1:112:A:ILE:N | 1:112:A:ILE:CA | 1:112:A:ILE:C | 5 | 10.27 | 1.3 | 10.76 |
| (1,175) | 1:94:A:GLU:N | 1:94:A:GLU:CA | 1:94:A:GLU:C | 1:95:A:ASN:N | 5 | 7.69 | 2.62 | 6.43 |
| (1,83) | 1:107:A:LYS:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 5 | 2.09 | 0.34 | 1.93 |
| (1,62) | 1:90:A:LEU:N | 1:90:A:LEU:CA | 1:90:A:LEU:C | 1:91:A:LYS:N | 5 | 1.85 | 0.54 | 2.06 |
| (1,169) | 1:86:A:LEU:N | 1:86:A:LEU:CA | 1:86:A:LEU:C | 1:87:A:LYS:N | 5 | 1.61 | 0.38 | 1.71 |
| (1,54) | 1:77:A:ILE:N | 1:77:A:ILE:CA | 1:77:A:ILE:C | 1:78:A:GLN:N | 5 | 1.32 | 0.15 | 1.35 |
| (1,33) | 1:56:A:GLU:C | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 4 | 1.68 | 0.17 | 1.68 |
| (1,27) | 1:47:A:GLU:C | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 4 | 1.32 | 0.24 | 1.32 |
| (1,91) | 1:33:A:VAL:C | 1:34:A:LYS:N | 1:34:A:LYS:CA | 1:34:A:LYS:C | 3 | 11.2 | 7.44 | 8.45 |
| (1,90) | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 1:18:A:TYR:N | 3 | 3.82 | 0.51 | 3.63 |
| (1,82) | 1:107:A:LYS:N | 1:107:A:LYS:CA | 1:107:A:LYS:C | 1:108:A:THR:N | 3 | 2.23 | 0.16 | 2.28 |
| (1,26) | 1:47:A:GLU:N | 1:47:A:GLU:CA | 1:47:A:GLU:C | 1:48:A:THR:N | 3 | 2.1 | 0.63 | 2.15 |
| (1,28) | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 1:49:A:GLU:N | 3 | 2.07 | 0.4 | 2.02 |
| (1,43) | 1:64:A:TYR:C | 1:65:A:LYS:N | 1:65:A:LYS:CA | 1:65:A:LYS:C | 3 | 1.64 | 0.46 | 1.31 |
| (1,87) | 1:109:A:MET:C | 1:110:A:THR:N | 1:110:A:THR:CA | 1:110:A:THR:C | 3 | 1.58 | 0.29 | 1.67 |
| (1,49) | 1:74:A:SER:C | 1:75:A:ILE:N | 1:75:A:ILE:CA | 1:75:A:ILE:C | 3 | 1.56 | 0.23 | 1.64 |
| (1,11) | 1:37:A:THR:C | 1:38:A:VAL:N | 1:38:A:VAL:CA | 1:38:A:VAL:C | 3 | 1.55 | 0.28 | 1.69 |
| (1,98) | 1:92:A:ARG:N | 1:92:A:ARG:CA | 1:92:A:ARG:C | 1:93:A:GLY:N | 3 | 1.54 | 0.33 | 1.33 |
| (1,50) | 1:75:A:ILE:N | 1:75:A:ILE:CA | 1:75:A:ILE:C | 1:76:A:GLU:N | 3 | 1.31 | 0.22 | 1.44 |
| (1,7) | 1:35:A:SER:C | 1:36:A:ALA:N | 1:36:A:ALA:CA | 1:36:A:ALA:C | 2 | 2.0 | 0.96 | 2.0 |
| (1,70) | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 1:100:A:TRP:N | 2 | 1.8 | 0.22 | 1.8 |
| (1,86) | 1:109:A:MET:N | 1:109:A:MET:CA | 1:109:A:MET:C | 1:110:A:THR:N | 2 | 1.7 | 0.15 | 1.7 |
| (1,65) | 1:96:A:GLY:C | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 2 | 1.42 | 0.42 | 1.42 |
| (1,72) | 1:100:A:TRP:N | 1:100:A:TRP:CA | 1:100:A:TRP:C | 1:101:A:GLU:N | 2 | 1.14 | 0.09 | 1.14 |

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 (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 1 | 146.65 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 20 | 143.26 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 5 | 137.78 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 8 | 137.45 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 4 | 125.81 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 11 | 111.24 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 18 | 107.46 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 19 | 36.81 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 13 | 35.7 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 6 | 33.69 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 12 | 31.07 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 7 | 29.71 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 9 | 27.22 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 17 | 26.48 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 14 | 25.27 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 15 | 23.81 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 2 | 23.17 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 3 | 23.07 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 10 | 22.63 |
| (1,91) | 1:33:A:VAL:C | 1:34:A:LYS:N | 1:34:A:LYS:CA | 1:34:A:LYS:C | 1 | 21.37 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 17 | 20.61 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 15 | 19.62 |
| (1,96) | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 1:85:A:PRO:N | 16 | 19.51 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 8 | 13.36 |
| (1,186) | 1:111:A:ARG:C | 1:112:A:ILE:N | 1:112:A:ILE:CA | 1:112:A:ILE:C | 16 | 11.86 |
| (1,175) | 1:94:A:GLU:N | 1:94:A:GLU:CA | 1:94:A:GLU:C | 1:95:A:ASN:N | 17 | 11.76 |
| (1,186) | 1:111:A:ARG:C | 1:112:A:ILE:N | 1:112:A:ILE:CA | 1:112:A:ILE:C | 8 | 10.87 |
| (1,186) | 1:111:A:ARG:C | 1:112:A:ILE:N | 1:112:A:ILE:CA | 1:112:A:ILE:C | 9 | 10.76 |
| (1,186) | 1:111:A:ARG:C | 1:112:A:ILE:N | 1:112:A:ILE:CA | 1:112:A:ILE:C | 12 | 9.86 |
| (1,175) | 1:94:A:GLU:N | 1:94:A:GLU:CA | 1:94:A:GLU:C | 1:95:A:ASN:N | 14 | 9.5 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 7 | 8.96 |
| (1,91) | 1:33:A:VAL:C | 1:34:A:LYS:N | 1:34:A:LYS:CA | 1:34:A:LYS:C | 17 | 8.45 |
| (1,89) | 1:16:A:PHE:C | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 7 | 8.07 |
| (1,186) | 1:111:A:ARG:C | 1:112:A:ILE:N | 1:112:A:ILE:CA | 1:112:A:ILE:C | 11 | 7.99 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 16 | 7.96 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 5 | 7.74 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 20 | 7.73 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 10 | 7.49 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 12 | 7.3 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 1 | 6.49 |
| (1,175) | 1:94:A:GLU:N | 1:94:A:GLU:CA | 1:94:A:GLU:C | 1:95:A:ASN:N | 6 | 6.43 |
| (1,175) | 1:94:A:GLU:N | 1:94:A:GLU:CA | 1:94:A:GLU:C | 1:95:A:ASN:N | 9 | 6.41 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 18 | 6.06 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 15 | 5.01 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 14 | 5.01 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 4 | 4.9 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 2 | 4.89 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 9 | 4.78 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 18 | 4.76 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 15 | 4.73 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 14 | 4.7 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 15 | 4.68 |
| (1,89) | 1:16:A:PHE:C | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 12 | 4.65 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 12 | 4.58 |
| (1,90) | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 1:18:A:TYR:N | 12 | 4.52 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 3 | 4.47 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 9 | 4.44 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 10 | 4.41 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 4 | 4.35 |
| (1,175) | 1:94:A:GLU:N | 1:94:A:GLU:CA | 1:94:A:GLU:C | 1:95:A:ASN:N | 13 | 4.34 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 10 | 4.23 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 13 | 4.21 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 16 | 4.2 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 17 | 4.16 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 6 | 4.15 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 3 | 4.14 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 10 | 4.1 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 12 | 4.09 |
| (1,89) | 1:16:A:PHE:C | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 18 | 4.05 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 4 | 4.04 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 16 | 3.94 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 10 | 3.8 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,91) | 1:33:A:VAL:C | 1:34:A:LYS:N | 1:34:A:LYS:CA | 1:34:A:LYS:C | 4 | 3.78 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 7 | 3.75 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 9 | 3.71 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 2 | 3.67 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 13 | 3.65 |
| (1,90) | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 1:18:A:TYR:N | 1 | 3.63 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 2 | 3.61 |
| (1,17) | 1:40:A:PHE:C | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 14 | 3.58 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 3 | 3.56 |
| (1,116) | 1:28:A:GLY:N | 1:28:A:GLY:CA | 1:28:A:GLY:C | 1:29:A:PRO:N | 1 | 3.54 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 12 | 3.52 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 20 | 3.52 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 17 | 3.5 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 3 | 3.47 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 11 | 3.46 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 2 | 3.41 |
| (1,84) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:MET:N | 3 | 3.4 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 6 | 3.35 |
| (1,90) | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 1:18:A:TYR:N | 18 | 3.32 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 1 | 3.31 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 10 | 3.28 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 18 | 3.22 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 12 | 3.21 |
| (1,89) | 1:16:A:PHE:C | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 10 | 3.2 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 17 | 3.2 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 6 | 3.1 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 3 | 3.09 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 15 | 3.02 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 15 | 3.02 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 18 | 3.0 |
| (1,80) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 1:107:A:LYS:N | 18 | 2.97 |
| (1,7) | 1:35:A:SER:C | 1:36:A:ALA:N | 1:36:A:ALA:CA | 1:36:A:ALA:C | 12 | 2.96 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 5 | 2.94 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 9 | 2.92 |
| (1,26) | 1:47:A:GLU:N | 1:47:A:GLU:CA | 1:47:A:GLU:C | 1:48:A:THR:N | 1 | 2.84 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 7 | 2.84 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 12 | 2.8 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 3 | 2.78 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 13 | 2.77 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 3 | 2.77 |
| (1,84) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:MET:N | 15 | 2.76 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 1 | 2.76 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 9 | 2.75 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 20 | 2.75 |
| (1,83) | 1:107:A:LYS:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 15 | 2.74 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 12 | 2.72 |
| (1,89) | 1:16:A:PHE:C | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 4 | 2.7 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 17 | 2.7 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 8 | 2.7 |
| (1,66) | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 1:98:A:LEU:N | 6 | 2.67 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 14 | 2.64 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 12 | 2.63 |
| (1,89) | 1:16:A:PHE:C | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 9 | 2.59 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 19 | 2.58 |
| (1,28) | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 1:49:A:GLU:N | 10 | 2.58 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 14 | 2.57 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 11 | 2.48 |
| (1,62) | 1:90:A:LEU:N | 1:90:A:LEU:CA | 1:90:A:LEU:C | 1:91:A:LYS:N | 3 | 2.47 |
| (1,34) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLN:N | 17 | 2.46 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 4 | 2.44 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 3 | 2.43 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 20 | 2.43 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1 | 2.41 |
| (1,82) | 1:107:A:LYS:N | 1:107:A:LYS:CA | 1:107:A:LYS:C | 1:108:A:THR:N | 9 | 2.4 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 8 | 2.39 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 8 | 2.39 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 15 | 2.39 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 15 | 2.35 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 2 | 2.35 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 20 | 2.34 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 16 | 2.33 |
| (1,84) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:MET:N | 9 | 2.32 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 7 | 2.3 |
| (1,43) | 1:64:A:TYR:C | 1:65:A:LYS:N | 1:65:A:LYS:CA | 1:65:A:LYS:C | 8 | 2.29 |
| (1,82) | 1:107:A:LYS:N | 1:107:A:LYS:CA | 1:107:A:LYS:C | 1:108:A:THR:N | 10 | 2.28 |
| (1,62) | 1:90:A:LEU:N | 1:90:A:LEU:CA | 1:90:A:LEU:C | 1:91:A:LYS:N | 14 | 2.28 |
| (1,116) | 1:28:A:GLY:N | 1:28:A:GLY:CA | 1:28:A:GLY:C | 1:29:A:PRO:N | 2 | 2.26 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 17 | 2.25 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 5 | 2.24 |
| (1,66) | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 1:98:A:LEU:N | 14 | 2.24 |
| (1,17) | 1:40:A:PHE:C | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 12 | 2.23 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 14 | 2.23 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 7 | 2.21 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 4 | 2.2 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 5 | 2.19 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 5 | 2.18 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 9 | 2.17 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 6 | 2.15 |
| (1,26) | 1:47:A:GLU:N | 1:47:A:GLU:CA | 1:47:A:GLU:C | 1:48:A:THR:N | 20 | 2.15 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 1 | 2.13 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 13 | 2.13 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 6 | 2.11 |
| (1,83) | 1:107:A:LYS:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 6 | 2.07 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 11 | 2.07 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 12 | 2.07 |
| (1,9) | 1:36:A:ALA:C | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 16 | 2.07 |
| (1,169) | 1:86:A:LEU:N | 1:86:A:LEU:CA | 1:86:A:LEU:C | 1:87:A:LYS:N | 7 | 2.06 |
| (1,62) | 1:90:A:LEU:N | 1:90:A:LEU:CA | 1:90:A:LEU:C | 1:91:A:LYS:N | 16 | 2.06 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 12 | 2.04 |
| (1,17) | 1:40:A:PHE:C | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 7 | 2.04 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 14 | 2.03 |
| (1,80) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 1:107:A:LYS:N | 7 | 2.03 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,70) | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 1:100:A:TRP:N | 17 | 2.03 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 6 | 2.03 |
| (1,28) | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 1:49:A:GLU:N | 13 | 2.02 |
| (1,82) | 1:107:A:LYS:N | 1:107:A:LYS:CA | 1:107:A:LYS:C | 1:108:A:THR:N | 4 | 2.01 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 4 | 2.01 |
| (1,98) | 1:92:A:ARG:N | 1:92:A:ARG:CA | 1:92:A:ARG:C | 1:93:A:GLY:N | 14 | 2.0 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 17 | 1.99 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 14 | 1.97 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 14 | 1.97 |
| (1,169) | 1:86:A:LEU:N | 1:86:A:LEU:CA | 1:86:A:LEU:C | 1:87:A:LYS:N | 9 | 1.96 |
| (1,34) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLN:N | 18 | 1.96 |
| (1,83) | 1:107:A:LYS:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 7 | 1.93 |
| (1,95) | 1:83:A:TYR:C | 1:84:A:TYR:N | 1:84:A:TYR:CA | 1:84:A:TYR:C | 2 | 1.92 |
| (1,33) | 1:56:A:GLU:C | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 5 | 1.92 |
| (1,177) | 1:95:A:ASN:N | 1:95:A:ASN:CA | 1:95:A:ASN:C | 1:96:A:GLY:N | 20 | 1.91 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 19 | 1.91 |
| (1,66) | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 1:98:A:LEU:N | 8 | 1.91 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 19 | 1.91 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 20 | 1.89 |
| (1,87) | 1:109:A:MET:C | 1:110:A:THR:N | 1:110:A:THR:CA | 1:110:A:THR:C | 6 | 1.88 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 11 | 1.87 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 17 | 1.87 |
| (1,83) | 1:107:A:LYS:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 2 | 1.86 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 18 | 1.86 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 5 | 1.86 |
| (1,86) | 1:109:A:MET:N | 1:109:A:MET:CA | 1:109:A:MET:C | 1:110:A:THR:N | 20 | 1.85 |
| (1,83) | 1:107:A:LYS:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 12 | 1.84 |
| (1,65) | 1:96:A:GLY:C | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 12 | 1.83 |
| (1,94) | 1:51:A:MET:N | 1:51:A:MET:CA | 1:51:A:MET:C | 1:52:A:GLU:N | 12 | 1.82 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 1 | 1.82 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 10 | 1.82 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 8 | 1.81 |
| (1,84) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:MET:N | 8 | 1.8 |
| (1,11) | 1:37:A:THR:C | 1:38:A:VAL:N | 1:38:A:VAL:CA | 1:38:A:VAL:C | 20 | 1.8 |
| (1,49) | 1:74:A:SER:C | 1:75:A:ILE:N | 1:75:A:ILE:CA | 1:75:A:ILE:C | 3 | 1.79 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 1 | 1.79 |
| (1,116) | 1:28:A:GLY:N | 1:28:A:GLY:CA | 1:28:A:GLY:C | 1:29:A:PRO:N | 10 | 1.78 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 3 | 1.76 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 19 | 1.75 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 12 | 1.74 |
| (1,89) | 1:16:A:PHE:C | 1:17:A:TYR:N | 1:17:A:TYR:CA | 1:17:A:TYR:C | 17 | 1.73 |
| (1,33) | 1:56:A:GLU:C | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 11 | 1.73 |
| (1,34) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLN:N | 6 | 1.72 |
| (1,169) | 1:86:A:LEU:N | 1:86:A:LEU:CA | 1:86:A:LEU:C | 1:87:A:LYS:N | 16 | 1.71 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 11 | 1.71 |
| (1,34) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLN:N | 1 | 1.71 |
| (1,9) | 1:36:A:ALA:C | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 4 | 1.71 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 2 | 1.7 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 8 | 1.69 |
| (1,11) | 1:37:A:THR:C | 1:38:A:VAL:N | 1:38:A:VAL:CA | 1:38:A:VAL:C | 16 | 1.69 |
| (1,87) | 1:109:A:MET:C | 1:110:A:THR:N | 1:110:A:THR:CA | 1:110:A:THR:C | 11 | 1.67 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 9 | 1.67 |
| (1,49) | 1:74:A:SER:C | 1:75:A:ILE:N | 1:75:A:ILE:CA | 1:75:A:ILE:C | 10 | 1.64 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 17 | 1.64 |
| (1,27) | 1:47:A:GLU:C | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 3 | 1.63 |
| (1,33) | 1:56:A:GLU:C | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 8 | 1.62 |
| (1,9) | 1:36:A:ALA:C | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 12 | 1.61 |
| (1,28) | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 1:49:A:GLU:N | 11 | 1.6 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 17 | 1.6 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 18 | 1.6 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 17 | 1.59 |
| (1,85) | 1:108:A:THR:C | 1:109:A:MET:N | 1:109:A:MET:CA | 1:109:A:MET:C | 6 | 1.58 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 11 | 1.58 |
| (1,70) | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 1:100:A:TRP:N | 6 | 1.58 |
| (1,66) | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 1:98:A:LEU:N | 12 | 1.58 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 10 | 1.57 |
| (1,86) | 1:109:A:MET:N | 1:109:A:MET:CA | 1:109:A:MET:C | 1:110:A:THR:N | 10 | 1.56 |
| (1,34) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLN:N | 12 | 1.56 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 11 | 1.55 |
| (1,75) | 1:101:A:GLU:C | 1:102:A:GLN:N | 1:102:A:GLN:CA | 1:102:A:GLN:C | 16 | 1.55 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 19 | 1.54 |
| (1,54) | 1:77:A:ILE:N | 1:77:A:ILE:CA | 1:77:A:ILE:C | 1:78:A:GLN:N | 18 | 1.53 |
| (1,22) | 1:45:A:VAL:N | 1:45:A:VAL:CA | 1:45:A:VAL:C | 1:46:A:VAL:N | 13 | 1.53 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 10 | 1.52 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 11 | 1.51 |
| (1,80) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 1:107:A:LYS:N | 16 | 1.51 |
| (1,78) | 1:105:A:GLN:N | 1:105:A:GLN:CA | 1:105:A:GLN:C | 1:106:A:ARG:N | 17 | 1.5 |
| (1,50) | 1:75:A:ILE:N | 1:75:A:ILE:CA | 1:75:A:ILE:C | 1:76:A:GLU:N | 13 | 1.49 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 11 | 1.49 |
| (1,27) | 1:47:A:GLU:C | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 14 | 1.47 |
| (1,33) | 1:56:A:GLU:C | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 19 | 1.46 |
| (1,50) | 1:75:A:ILE:N | 1:75:A:ILE:CA | 1:75:A:ILE:C | 1:76:A:GLU:N | 15 | 1.44 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 5 | 1.43 |
| (1,80) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 1:107:A:LYS:N | 11 | 1.43 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 11 | 1.43 |
| (1,79) | 1:105:A:GLN:C | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 10 | 1.41 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 3 | 1.41 |
| (1,54) | 1:77:A:ILE:N | 1:77:A:ILE:CA | 1:77:A:ILE:C | 1:78:A:GLN:N | 3 | 1.41 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 20 | 1.4 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 5 | 1.4 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 14 | 1.4 |
| (1,62) | 1:90:A:LEU:N | 1:90:A:LEU:CA | 1:90:A:LEU:C | 1:91:A:LYS:N | 18 | 1.38 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 10 | 1.38 |
| (1,18) | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1:42:A:GLU:N | 1 | 1.36 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 9 | 1.36 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 13 | 1.36 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 20 | 1.36 |
| (1,54) | 1:77:A:ILE:N | 1:77:A:ILE:CA | 1:77:A:ILE:C | 1:78:A:GLN:N | 19 | 1.35 |
| (1,32) | 1:50:A:VAL:N | 1:50:A:VAL:CA | 1:50:A:VAL:C | 1:51:A:MET:N | 13 | 1.35 |
| (1,17) | 1:40:A:PHE:C | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 1 | 1.35 |
| (1,98) | 1:92:A:ARG:N | 1:92:A:ARG:CA | 1:92:A:ARG:C | 1:93:A:GLY:N | 20 | 1.33 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 9 | 1.33 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,17) | 1:40:A:PHE:C | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 16 | 1.33 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 5 | 1.33 |
| (1,55) | 1:77:A:ILE:C | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 9 | 1.32 |
| (1,116) | 1:28:A:GLY:N | 1:28:A:GLY:CA | 1:28:A:GLY:C | 1:29:A:PRO:N | 16 | 1.31 |
| (1,84) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:MET:N | 11 | 1.31 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 16 | 1.31 |
| (1,43) | 1:64:A:TYR:C | 1:65:A:LYS:N | 1:65:A:LYS:CA | 1:65:A:LYS:C | 5 | 1.31 |
| (1,43) | 1:64:A:TYR:C | 1:65:A:LYS:N | 1:65:A:LYS:CA | 1:65:A:LYS:C | 18 | 1.31 |
| (1,26) | 1:47:A:GLU:N | 1:47:A:GLU:CA | 1:47:A:GLU:C | 1:48:A:THR:N | 7 | 1.31 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 8 | 1.31 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 2 | 1.3 |
| (1,17) | 1:40:A:PHE:C | 1:41:A:THR:N | 1:41:A:THR:CA | 1:41:A:THR:C | 10 | 1.29 |
| (1,98) | 1:92:A:ARG:N | 1:92:A:ARG:CA | 1:92:A:ARG:C | 1:93:A:GLY:N | 7 | 1.28 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 1 | 1.28 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 2 | 1.28 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 20 | 1.26 |
| (1,34) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLN:N | 10 | 1.26 |
| (1,19) | 1:43:A:ASP:C | 1:44:A:GLU:N | 1:44:A:GLU:CA | 1:44:A:GLU:C | 19 | 1.26 |
| (1,5) | 1:21:A:TRP:C | 1:22:A:ASP:N | 1:22:A:ASP:CA | 1:22:A:ASP:C | 2 | 1.26 |
| (1,47) | 1:68:A:SER:C | 1:69:A:GLN:N | 1:69:A:GLN:CA | 1:69:A:GLN:C | 18 | 1.25 |
| (1,84) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:MET:N | 13 | 1.24 |
| (1,80) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 1:107:A:LYS:N | 6 | 1.24 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 19 | 1.24 |
| (1,66) | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 1:98:A:LEU:N | 7 | 1.24 |
| (1,49) | 1:74:A:SER:C | 1:75:A:ILE:N | 1:75:A:ILE:CA | 1:75:A:ILE:C | 7 | 1.24 |
| (1,72) | 1:100:A:TRP:N | 1:100:A:TRP:CA | 1:100:A:TRP:C | 1:101:A:GLU:N | 3 | 1.23 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 9 | 1.22 |
| (1,80) | 1:106:A:ARG:N | 1:106:A:ARG:CA | 1:106:A:ARG:C | 1:107:A:LYS:N | 4 | 1.2 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 17 | 1.2 |
| (1,87) | 1:109:A:MET:C | 1:110:A:THR:N | 1:110:A:THR:CA | 1:110:A:THR:C | 16 | 1.19 |
| (1,56) | 1:78:A:GLN:N | 1:78:A:GLN:CA | 1:78:A:GLN:C | 1:79:A:TYR:N | 11 | 1.19 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 16 | 1.19 |
| (1,167) | 1:85:A:PRO:N | 1:85:A:PRO:CA | 1:85:A:PRO:C | 1:86:A:LEU:N | 4 | 1.18 |
| (1,169) | 1:86:A:LEU:N | 1:86:A:LEU:CA | 1:86:A:LEU:C | 1:87:A:LYS:N | 12 | 1.17 |
| (1,68) | 1:98:A:LEU:N | 1:98:A:LEU:CA | 1:98:A:LEU:C | 1:99:A:ILE:N | 13 | 1.17 |
| (1,169) | 1:86:A:LEU:N | 1:86:A:LEU:CA | 1:86:A:LEU:C | 1:87:A:LYS:N | 2 | 1.16 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 7 | 1.16 |
| (1,27) | 1:47:A:GLU:C | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 10 | 1.16 |
| (1,136) | 1:54:A:ARG:N | 1:54:A:ARG:CA | 1:54:A:ARG:C | 1:55:A:GLY:N | 13 | 1.15 |
| (1,54) | 1:77:A:ILE:N | 1:77:A:ILE:CA | 1:77:A:ILE:C | 1:78:A:GLN:N | 8 | 1.15 |
| (1,11) | 1:37:A:THR:C | 1:38:A:VAL:N | 1:38:A:VAL:CA | 1:38:A:VAL:C | 18 | 1.15 |
| (1,54) | 1:77:A:ILE:N | 1:77:A:ILE:CA | 1:77:A:ILE:C | 1:78:A:GLN:N | 11 | 1.14 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 8 | 1.13 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 5 | 1.13 |
| (1,9) | 1:36:A:ALA:C | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 15 | 1.13 |
| (1,69) | 1:98:A:LEU:C | 1:99:A:ILE:N | 1:99:A:ILE:CA | 1:99:A:ILE:C | 8 | 1.11 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 13 | 1.11 |
| (1,9) | 1:36:A:ALA:C | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 11 | 1.11 |
| (1,9) | 1:36:A:ALA:C | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 19 | 1.1 |
| (1,116) | 1:28:A:GLY:N | 1:28:A:GLY:CA | 1:28:A:GLY:C | 1:29:A:PRO:N | 3 | 1.09 |
| (1,84) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:MET:N | 17 | 1.09 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,10) | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 1:38:A:VAL:N | 4 | 1.09 |
| (1,29) | 1:48:A:THR:C | 1:49:A:GLU:N | 1:49:A:GLU:CA | 1:49:A:GLU:C | 2 | 1.08 |
| (1,62) | 1:90:A:LEU:N | 1:90:A:LEU:CA | 1:90:A:LEU:C | 1:91:A:LYS:N | 12 | 1.07 |
| (1,116) | 1:28:A:GLY:N | 1:28:A:GLY:CA | 1:28:A:GLY:C | 1:29:A:PRO:N | 11 | 1.05 |
| (1,72) | 1:100:A:TRP:N | 1:100:A:TRP:CA | 1:100:A:TRP:C | 1:101:A:GLU:N | 17 | 1.05 |
| (1,34) | 1:57:A:VAL:N | 1:57:A:VAL:CA | 1:57:A:VAL:C | 1:58:A:GLN:N | 16 | 1.05 |
| (1,27) | 1:47:A:GLU:C | 1:48:A:THR:N | 1:48:A:THR:CA | 1:48:A:THR:C | 9 | 1.03 |
| (1,15) | 1:39:A:THR:C | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 16 | 1.03 |
| (1,7) | 1:35:A:SER:C | 1:36:A:ALA:N | 1:36:A:ALA:CA | 1:36:A:ALA:C | 8 | 1.03 |
| (1,16) | 1:40:A:PHE:N | 1:40:A:PHE:CA | 1:40:A:PHE:C | 1:41:A:THR:N | 3 | 1.02 |
| (1,60) | 1:89:A:THR:N | 1:89:A:THR:CA | 1:89:A:THR:C | 1:90:A:LEU:N | 18 | 1.01 |
| (1,50) | 1:75:A:ILE:N | 1:75:A:ILE:CA | 1:75:A:ILE:C | 1:76:A:GLU:N | 20 | 1.01 |
| (1,66) | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 1:98:A:LEU:N | 13 | 1.0 |
| (1,65) | 1:96:A:GLY:C | 1:97:A:THR:N | 1:97:A:THR:CA | 1:97:A:THR:C | 6 | 1.0 |
| (1,9) | 1:36:A:ALA:C | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 1 | 1.0 |