



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:29 PM BST

PDB ID : 2JTC
Title : 3D structure and backbone dynamics of SPE B
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Deposited on : 2007-07-26

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

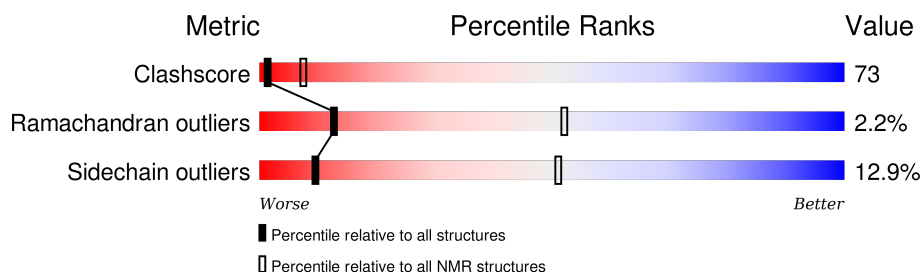
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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 | 114402 | 11133 |
| Ramachandran outliers | 111179 | 9975 |
| Sidechain outliers | 111093 | 9958 |

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 | 253 | |

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 5 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|---|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:4-A:31, A:37-A:212, A:245-A:253 (213) | 0.21 | 8 |

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 1 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3782 atoms, of which 1833 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Streptopain.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
| 1 | A | 253 | Total | C | H | N | O | S | 0 |
| | | | 3782 | 1227 | 1833 | 343 | 375 | 4 | |

There is a discrepancy between the modelled and reference sequences:

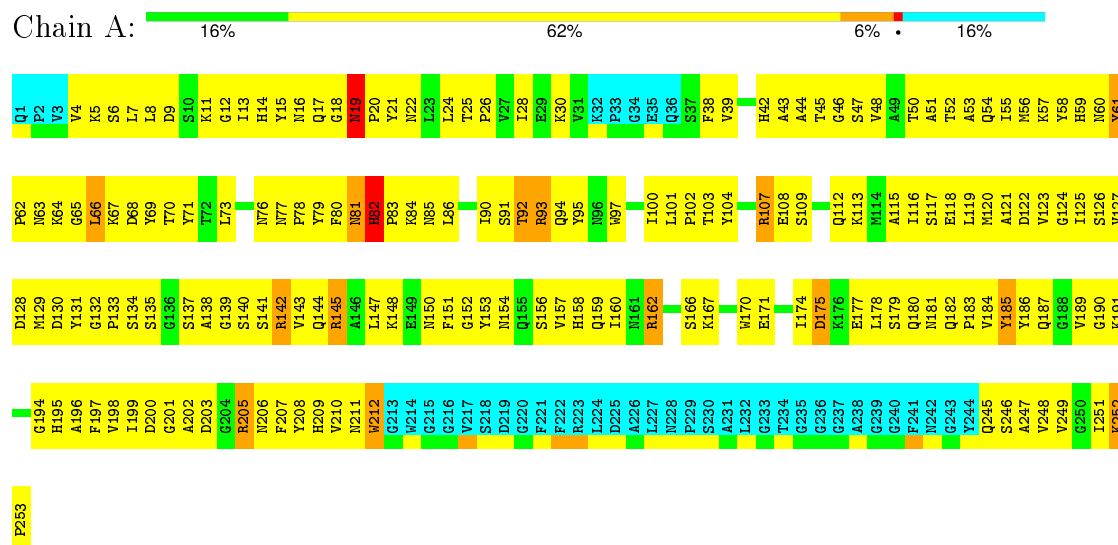
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|------------|
| A | 47 | SER | CYS | ENGINEERED | UNP P0C0J1 |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Streptopain

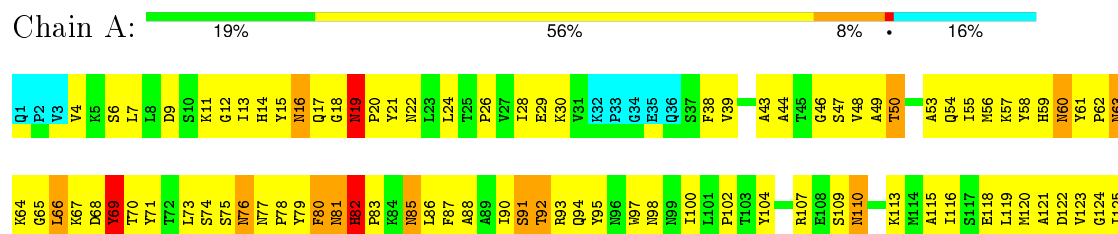


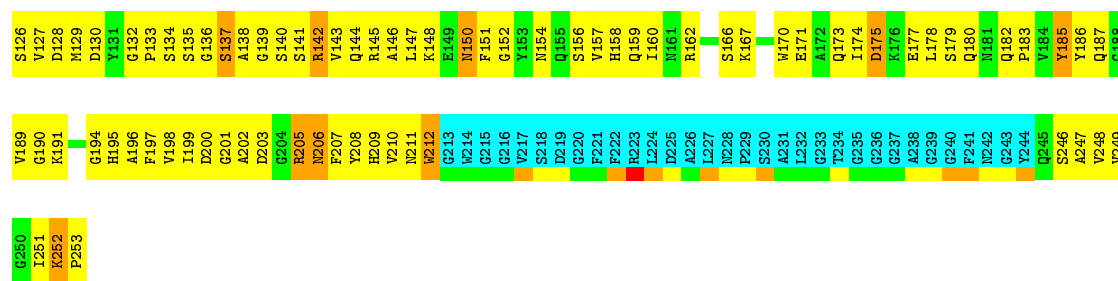
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Streptopain

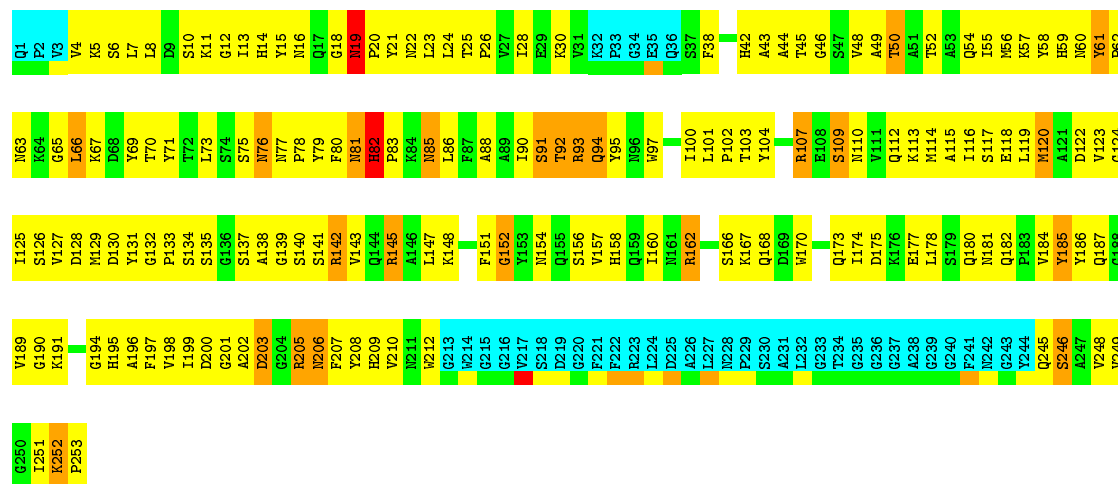




4.2.2 Score per residue for model 2

- Molecule 1: Streptopain

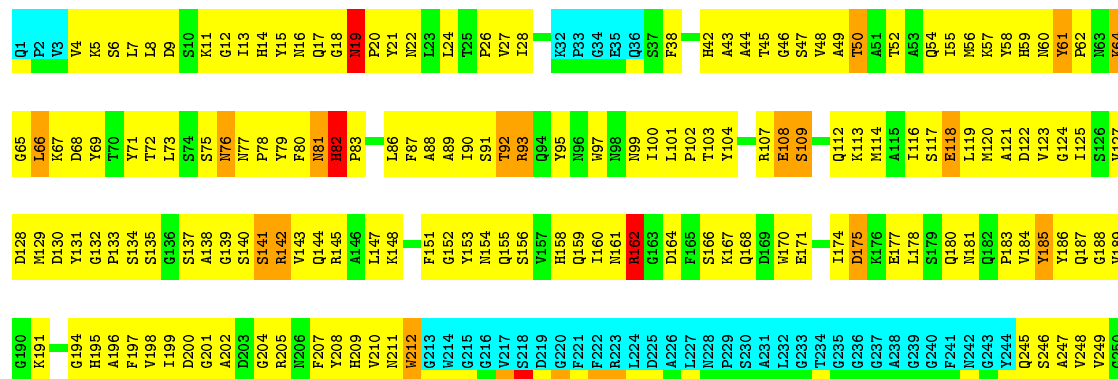
Chain A: 21% 54% 9% 16%



4.2.3 Score per residue for model 3

- Molecule 1: Streptopain

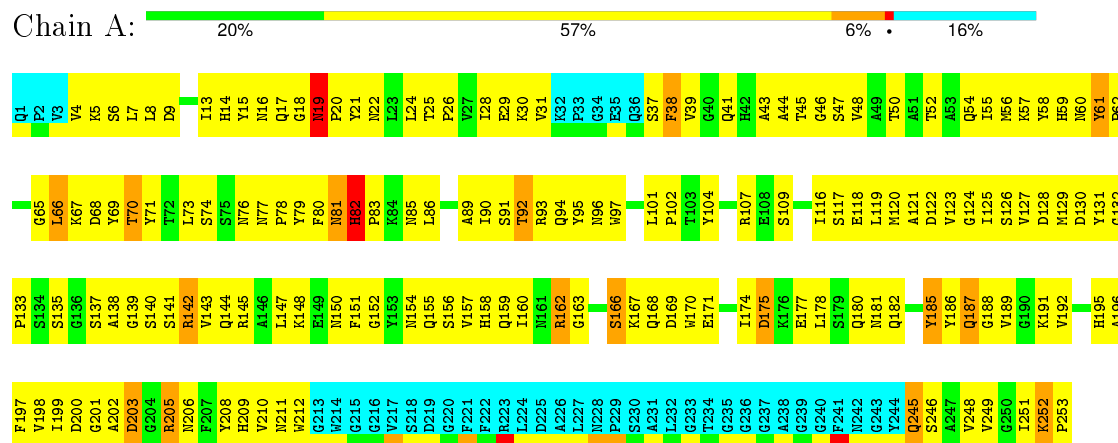
Chain A: 18% 58% 7% 16%



I251
K252
P253

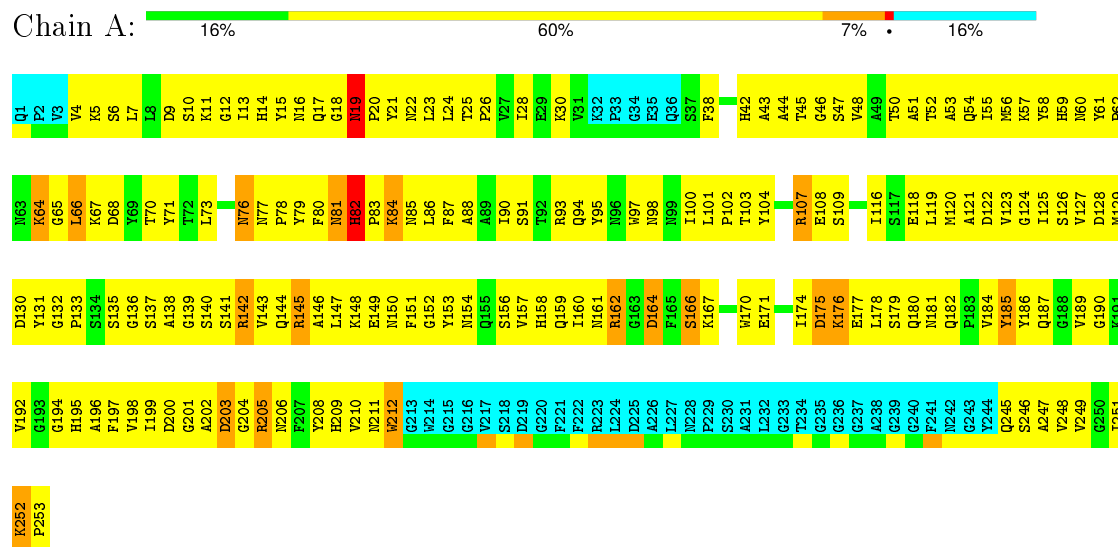
4.2.4 Score per residue for model 4

- Molecule 1: Streptopain



4.2.5 Score per residue for model 5

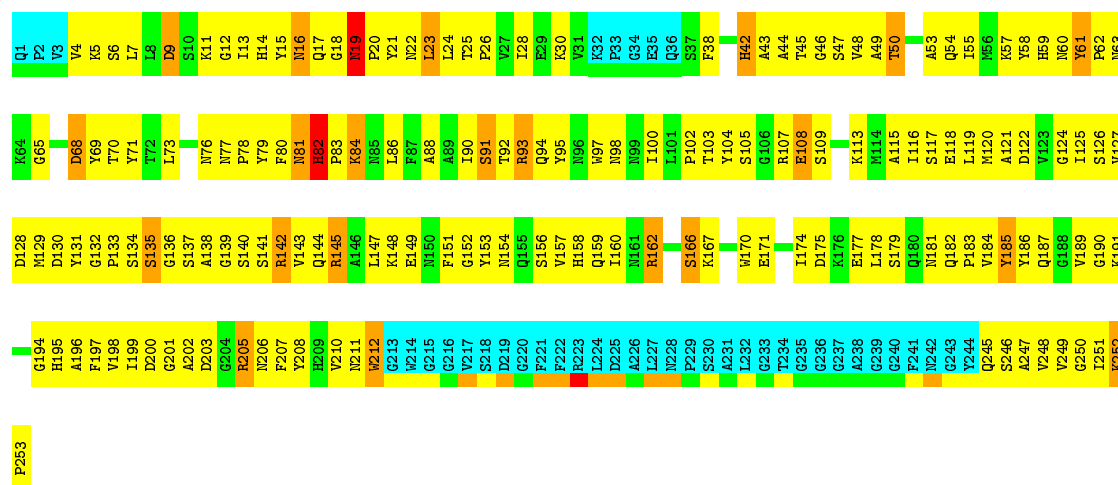
- Molecule 1: Streptopain



4.2.6 Score per residue for model 6

- Molecule 1: Streptopain

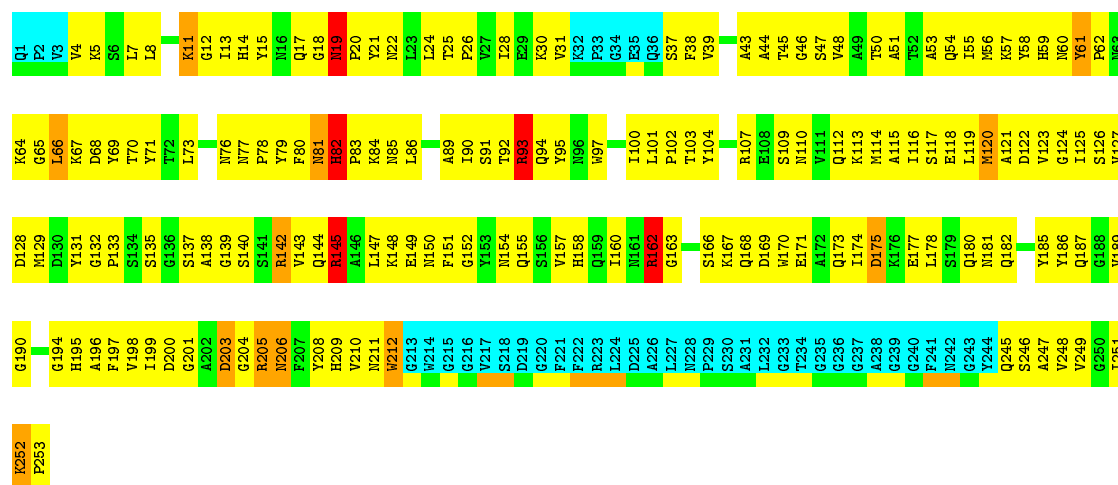




4.2.7 Score per residue for model 7

- Molecule 1: Streptopain

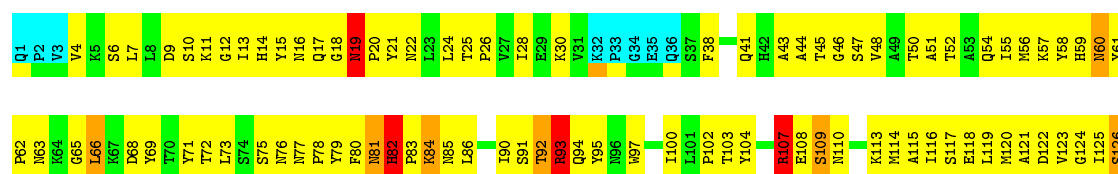
Chain A: 19% 58% 5% 16%

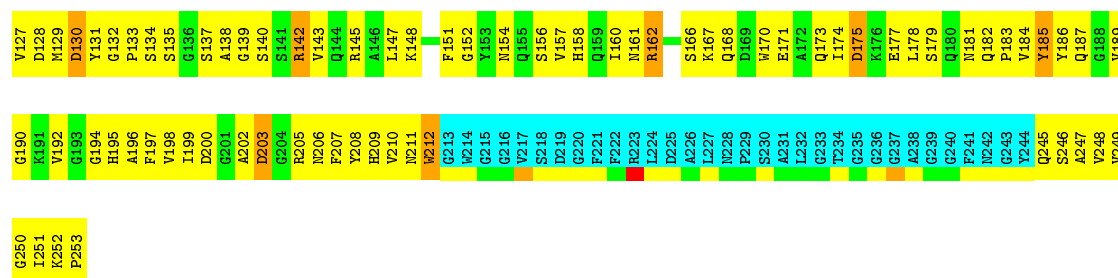


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Streptopain

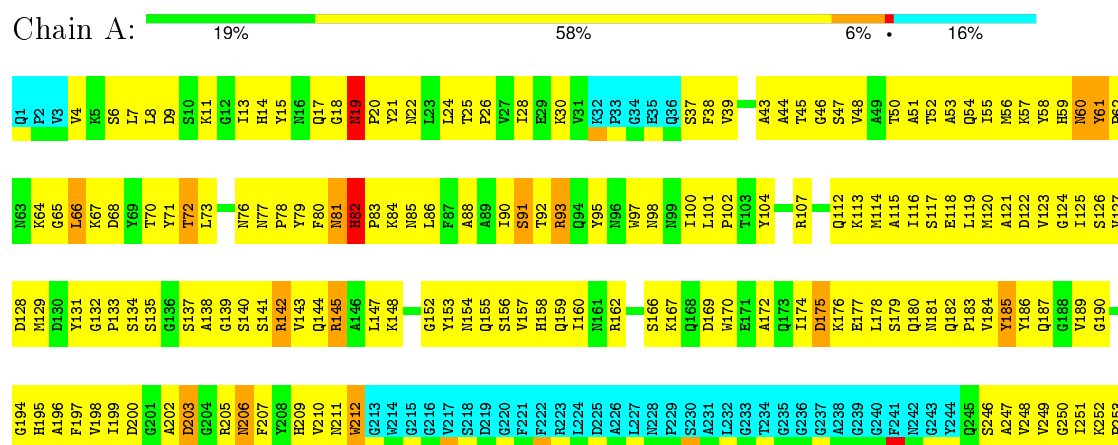
Chain A: 19% 58% 6% 16%





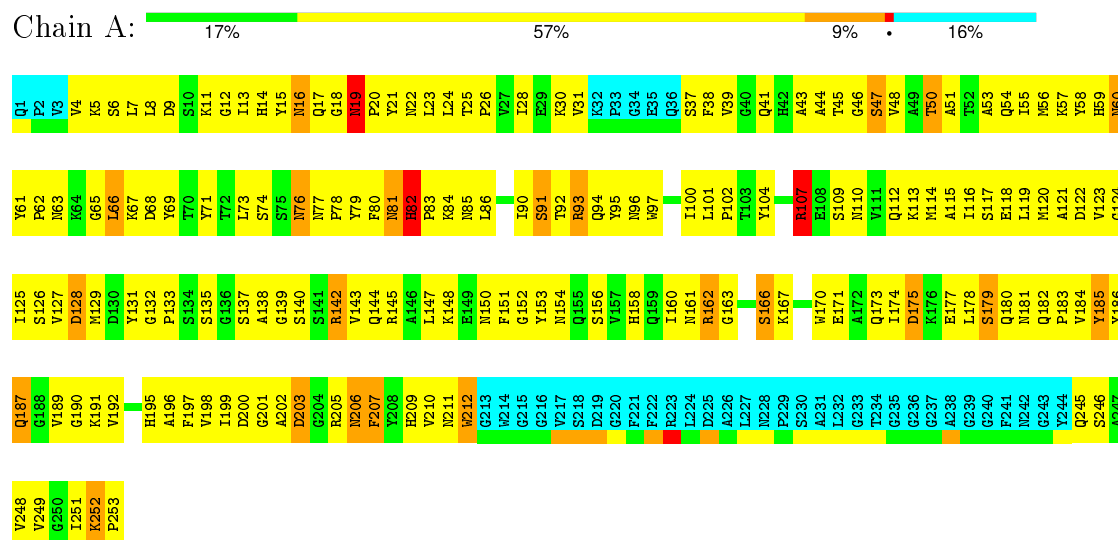
4.2.9 Score per residue for model 9

- Molecule 1: Streptopain



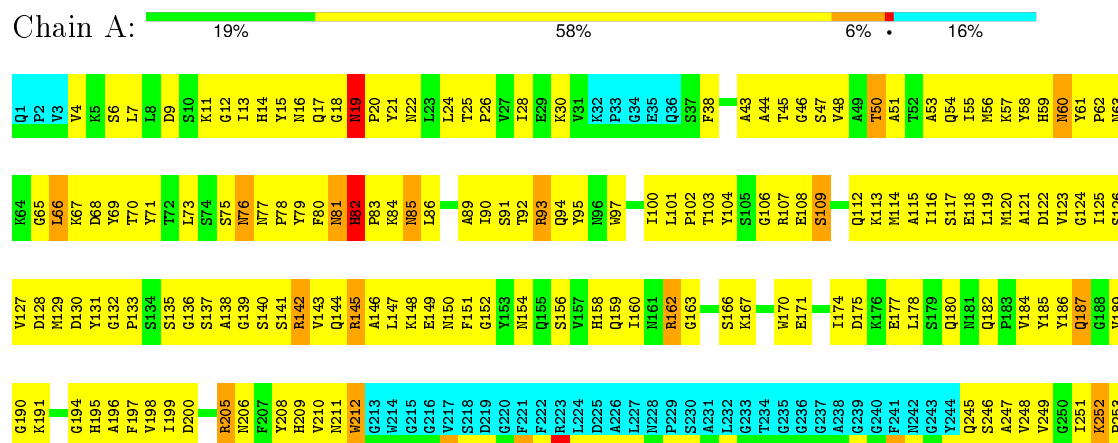
4.2.10 Score per residue for model 10

- Molecule 1: Streptopain



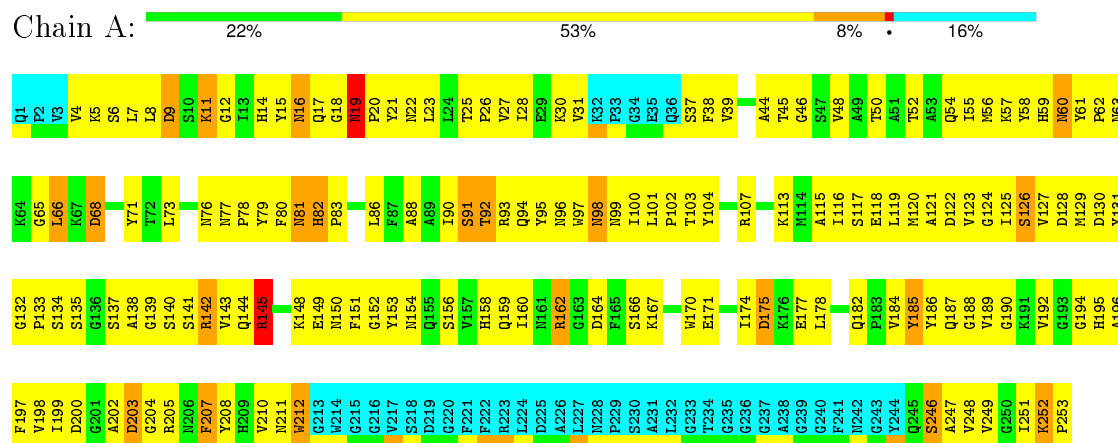
4.2.11 Score per residue for model 11

- Molecule 1: Streptopain



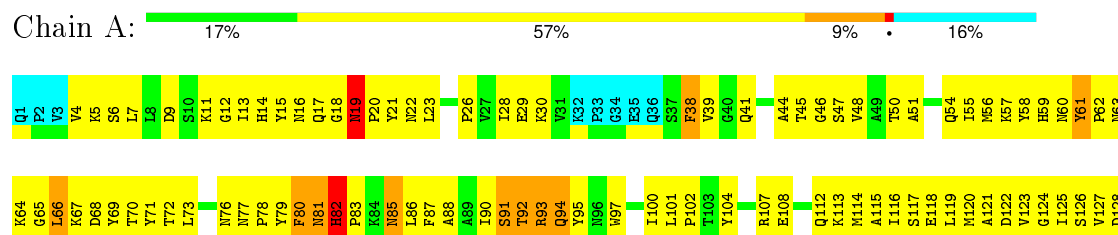
4.2.12 Score per residue for model 12

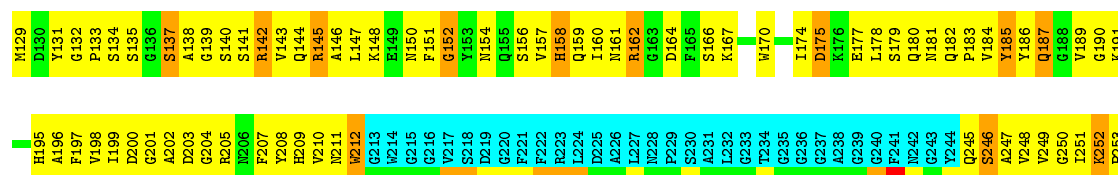
- Molecule 1: Streptopain



4.2.13 Score per residue for model 13

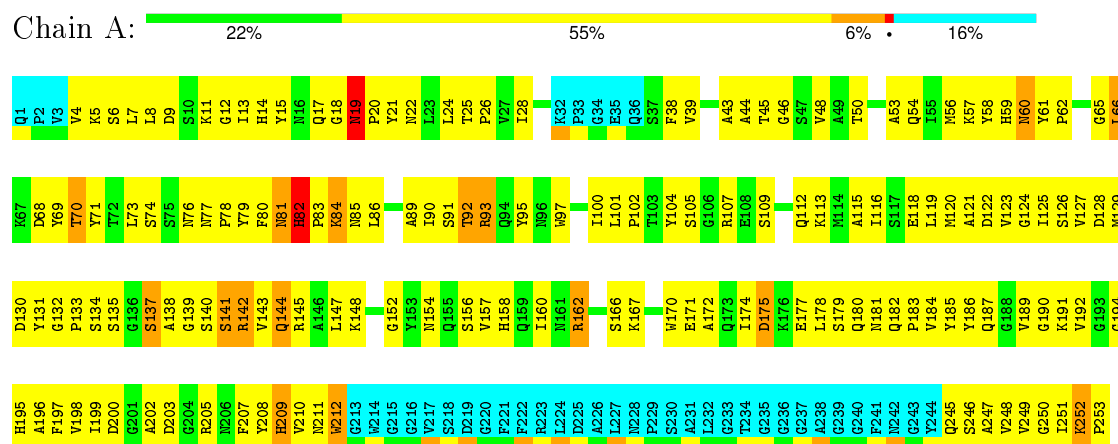
- Molecule 1: Streptopain





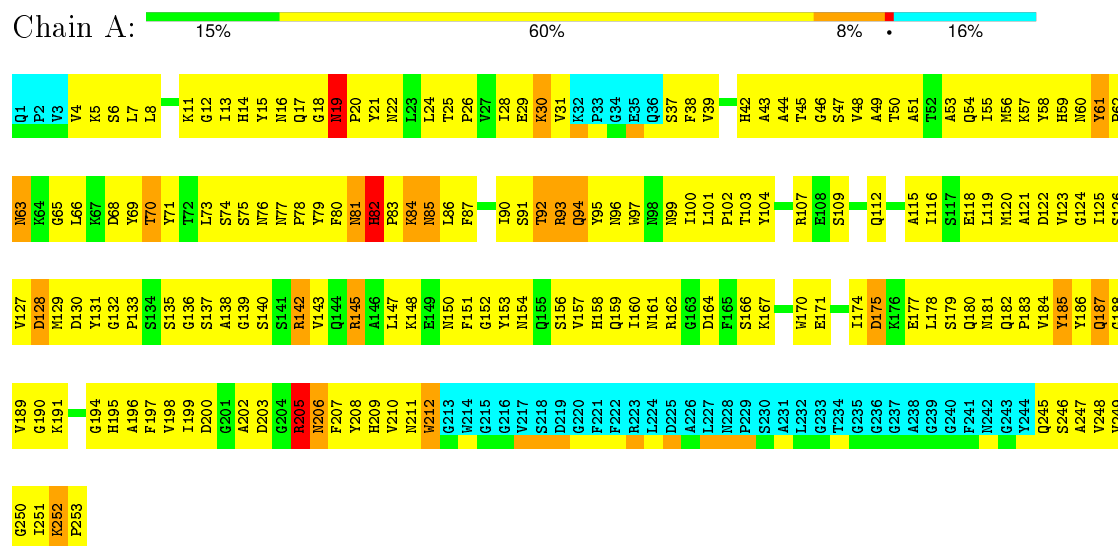
4.2.14 Score per residue for model 14

- Molecule 1: Streptopain



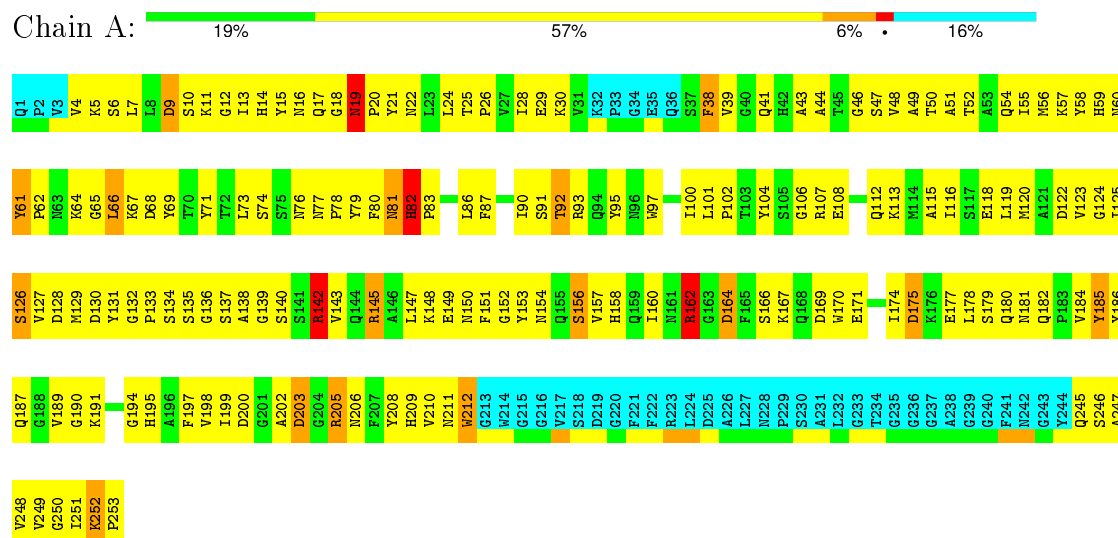
4.2.15 Score per residue for model 15

- Molecule 1: Streptopain



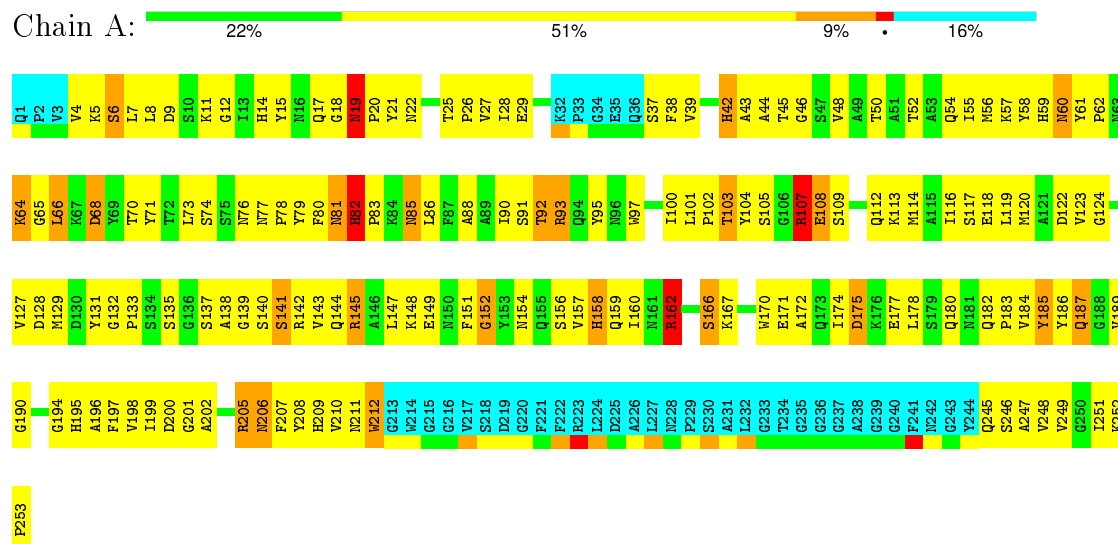
4.2.16 Score per residue for model 16

- Molecule 1: Streptopain



4.2.17 Score per residue for model 17

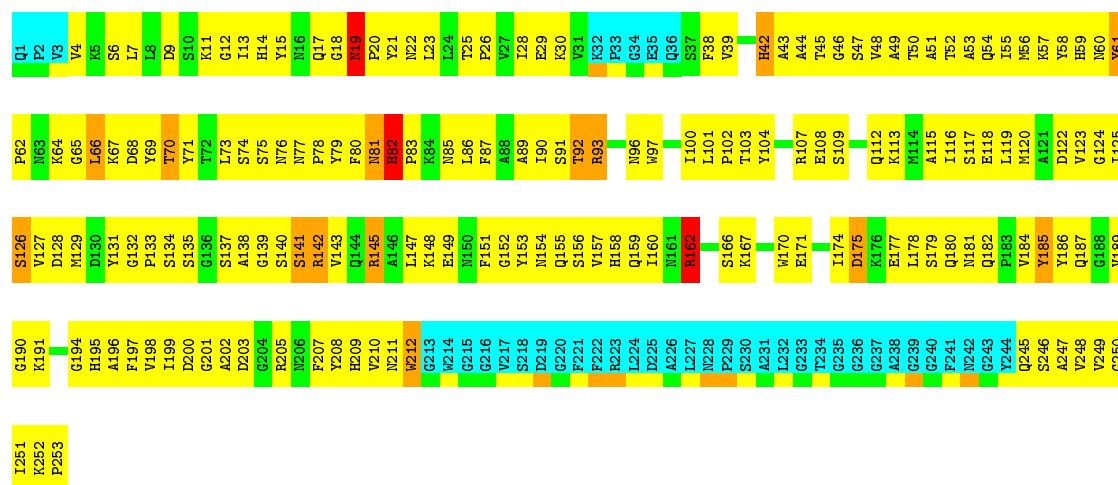
- Molecule 1: Streptopain



4.2.18 Score per residue for model 18

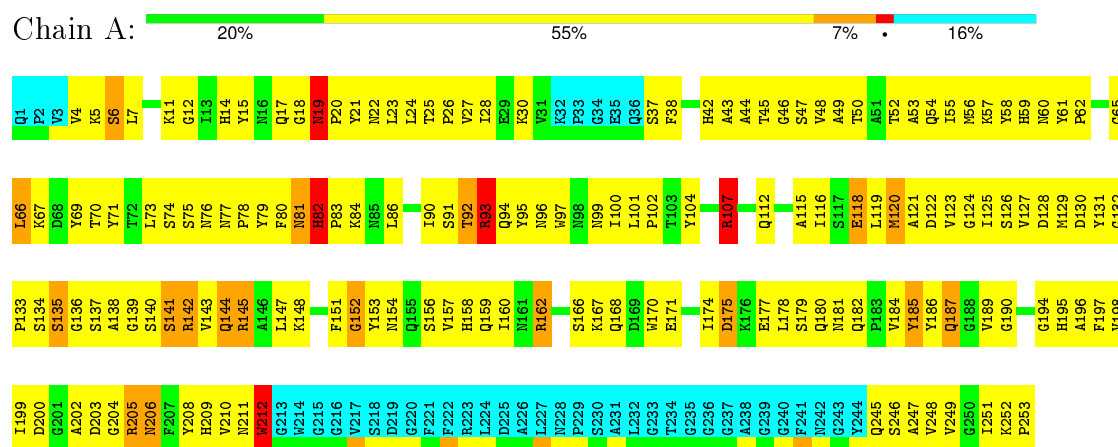
- Molecule 1: Streptopain





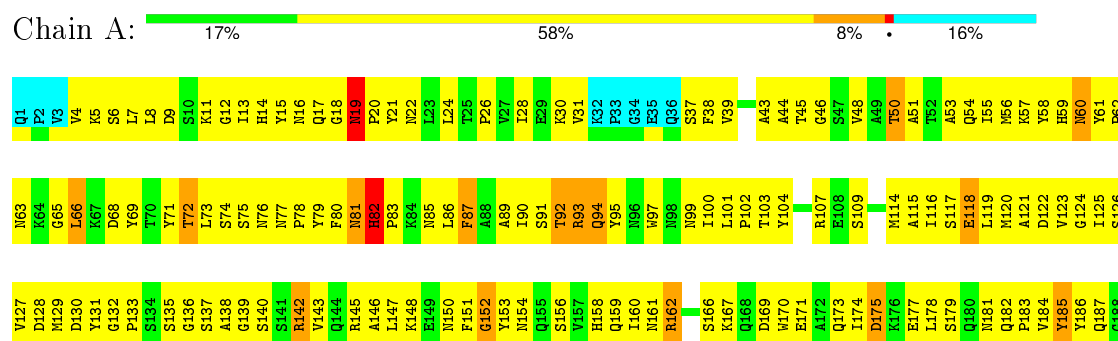
4.2.19 Score per residue for model 19

- Molecule 1: Streptopain



4.2.20 Score per residue for model 20

- Molecule 1: Streptopain



[illegible]

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry 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 |
|---------------|----------------|---------|
| X-PLOR | refinement | 3.185 |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------------|-------------|---------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.98±0.00 | 0±0/1712 (0.0±0.0%) | 0.96±0.01 | 0±0/2321 (0.0±0.0%) |
| All | All | 0.98 | 0/34240 (0.0%) | 0.96 | 4/46420 (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 | 5.5±0.7 |
| All | All | 0 | 110 |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 69 | TYR | CB-CG-CD1 | -6.45 | 117.13 | 121.00 | 1 | 1 |
| 1 | A | 38 | PHE | CB-CG-CD2 | -5.68 | 116.83 | 120.80 | 16 | 3 |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 205 | ARG | Sidechain | 20 |
| 1 | A | 145 | ARG | Sidechain | 20 |
| 1 | A | 107 | ARG | Sidechain | 20 |
| 1 | A | 142 | ARG | Sidechain | 19 |
| 1 | A | 162 | ARG | Sidechain | 17 |
| 1 | A | 93 | ARG | Sidechain | 14 |

6.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 1670 | 1580 | 1599 | 240±13 |
| All | All | 33400 | 31600 | 31980 | 4801 |

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 73.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:55:ILE:HG21 | 1:A:251:ILE:HD13 | 1.04 | 1.28 | 16 | 4 |
| 1:A:116:ILE:HD11 | 1:A:120:MET:HE2 | 0.98 | 1.34 | 18 | 2 |
| 1:A:160:ILE:HD12 | 1:A:170:TRP:CH2 | 0.97 | 1.94 | 9 | 6 |
| 1:A:55:ILE:HD11 | 1:A:198:VAL:HG22 | 0.96 | 1.34 | 4 | 18 |
| 1:A:174:ILE:HG23 | 1:A:184:VAL:HG21 | 0.93 | 1.41 | 8 | 14 |
| 1:A:158:HIS:CE1 | 1:A:249:VAL:HG23 | 0.93 | 1.98 | 1 | 10 |
| 1:A:66:LEU:HD12 | 1:A:152:GLY:HA3 | 0.92 | 1.41 | 3 | 19 |
| 1:A:143:VAL:HG21 | 1:A:185:TYR:CE2 | 0.89 | 2.02 | 4 | 19 |
| 1:A:55:ILE:CD1 | 1:A:198:VAL:HG22 | 0.89 | 1.98 | 2 | 16 |
| 1:A:45:THR:HG21 | 1:A:120:MET:SD | 0.88 | 2.08 | 7 | 13 |
| 1:A:174:ILE:HD13 | 1:A:199:ILE:CD1 | 0.87 | 1.99 | 4 | 3 |
| 1:A:19:ASN:ND2 | 1:A:20:PRO:HD2 | 0.85 | 1.85 | 18 | 1 |
| 1:A:123:VAL:O | 1:A:127:VAL:HG22 | 0.84 | 1.70 | 14 | 14 |
| 1:A:160:ILE:HD12 | 1:A:170:TRP:CZ3 | 0.84 | 2.07 | 6 | 17 |
| 1:A:185:TYR:CD1 | 1:A:248:VAL:HG23 | 0.83 | 2.08 | 12 | 14 |
| 1:A:184:VAL:HG13 | 1:A:249:VAL:HG12 | 0.81 | 1.50 | 14 | 7 |
| 1:A:138:ALA:HB3 | 1:A:142:ARG:CG | 0.80 | 2.06 | 17 | 13 |
| 1:A:69:TYR:CZ | 1:A:125:ILE:HG23 | 0.80 | 2.11 | 1 | 1 |
| 1:A:69:TYR:CE1 | 1:A:125:ILE:CG2 | 0.79 | 2.65 | 1 | 1 |
| 1:A:197:PHE:CD1 | 1:A:210:VAL:HG13 | 0.79 | 2.12 | 17 | 15 |
| 1:A:210:VAL:HG11 | 1:A:212:TRP:CZ3 | 0.79 | 2.12 | 6 | 1 |
| 1:A:69:TYR:CD1 | 1:A:69:TYR:C | 0.79 | 2.56 | 1 | 1 |
| 1:A:4:VAL:HG21 | 1:A:178:LEU:HB2 | 0.79 | 1.53 | 4 | 1 |
| 1:A:197:PHE:CD2 | 1:A:210:VAL:HG13 | 0.78 | 2.13 | 9 | 2 |
| 1:A:116:ILE:CD1 | 1:A:119:LEU:HD23 | 0.78 | 2.08 | 12 | 20 |
| 1:A:24:LEU:HD12 | 1:A:118:GLU:N | 0.77 | 1.93 | 14 | 14 |
| 1:A:138:ALA:HB3 | 1:A:142:ARG:HG2 | 0.77 | 1.55 | 1 | 11 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:38:PHE:CD2 | 1:A:133:PRO:HG3 | 0.76 | 2.16 | 16 | 10 |
| 1:A:44:ALA:HB3 | 1:A:135:SER:OG | 0.76 | 1.80 | 4 | 3 |
| 1:A:174:ILE:HG21 | 1:A:199:ILE:HD13 | 0.75 | 1.57 | 20 | 11 |
| 1:A:90:ILE:HD12 | 1:A:150:ASN:CG | 0.75 | 2.02 | 1 | 1 |
| 1:A:202:ALA:CB | 1:A:208:TYR:CE1 | 0.74 | 2.70 | 13 | 1 |
| 1:A:89:ALA:HB1 | 1:A:92:THR:HG23 | 0.74 | 1.57 | 18 | 2 |
| 1:A:21:TYR:HB3 | 1:A:120:MET:SD | 0.74 | 2.22 | 2 | 14 |
| 1:A:18:GLY:O | 1:A:19:ASN:O | 0.73 | 2.05 | 15 | 19 |
| 1:A:19:ASN:HB3 | 1:A:20:PRO:CD | 0.73 | 2.14 | 11 | 19 |
| 1:A:73:LEU:HD21 | 1:A:77:ASN:ND2 | 0.72 | 2.00 | 8 | 20 |
| 1:A:142:ARG:NH2 | 1:A:143:VAL:HG23 | 0.72 | 1.99 | 16 | 1 |
| 1:A:158:HIS:NE2 | 1:A:249:VAL:HG23 | 0.72 | 1.98 | 11 | 19 |
| 1:A:93:ARG:HE | 1:A:122:ASP:CG | 0.72 | 1.86 | 9 | 10 |
| 1:A:138:ALA:HB3 | 1:A:142:ARG:HG3 | 0.72 | 1.60 | 12 | 7 |
| 1:A:210:VAL:HG11 | 1:A:212:TRP:CE2 | 0.72 | 2.18 | 18 | 5 |
| 1:A:20:PRO:HA | 1:A:23:LEU:HD12 | 0.72 | 1.61 | 6 | 6 |
| 1:A:38:PHE:CD2 | 1:A:133:PRO:CG | 0.72 | 2.72 | 13 | 3 |
| 1:A:174:ILE:HG23 | 1:A:184:VAL:CG2 | 0.71 | 2.12 | 11 | 9 |
| 1:A:28:ILE:HD11 | 1:A:132:GLY:C | 0.71 | 2.04 | 17 | 17 |
| 1:A:170:TRP:NE1 | 1:A:174:ILE:HD11 | 0.71 | 2.01 | 4 | 2 |
| 1:A:19:ASN:HB3 | 1:A:20:PRO:HD2 | 0.71 | 1.62 | 10 | 19 |
| 1:A:72:THR:HG23 | 1:A:85:ASN:OD1 | 0.71 | 1.85 | 9 | 2 |
| 1:A:142:ARG:HB2 | 1:A:142:ARG:CZ | 0.71 | 2.15 | 16 | 1 |
| 1:A:89:ALA:HB1 | 1:A:92:THR:CG2 | 0.71 | 2.15 | 18 | 2 |
| 1:A:197:PHE:CD2 | 1:A:212:TRP:CZ3 | 0.70 | 2.79 | 15 | 9 |
| 1:A:69:TYR:CG | 1:A:70:THR:N | 0.70 | 2.60 | 1 | 1 |
| 1:A:66:LEU:N | 1:A:66:LEU:HD23 | 0.70 | 2.02 | 15 | 1 |
| 1:A:139:GLY:O | 1:A:142:ARG:NH2 | 0.69 | 2.25 | 16 | 1 |
| 1:A:19:ASN:ND2 | 1:A:20:PRO:CD | 0.69 | 2.55 | 18 | 1 |
| 1:A:66:LEU:HD12 | 1:A:152:GLY:CA | 0.69 | 2.17 | 4 | 19 |
| 1:A:4:VAL:HG11 | 1:A:178:LEU:HB3 | 0.69 | 1.64 | 4 | 17 |
| 1:A:186:TYR:CD1 | 1:A:197:PHE:CZ | 0.69 | 2.79 | 18 | 16 |
| 1:A:142:ARG:HH22 | 1:A:143:VAL:HG23 | 0.69 | 1.48 | 16 | 1 |
| 1:A:186:TYR:CD2 | 1:A:247:ALA:HB2 | 0.68 | 2.23 | 16 | 5 |
| 1:A:71:TYR:CZ | 1:A:86:LEU:HD13 | 0.68 | 2.24 | 9 | 17 |
| 1:A:186:TYR:CG | 1:A:197:PHE:CZ | 0.68 | 2.82 | 4 | 11 |
| 1:A:174:ILE:HD13 | 1:A:199:ILE:HD12 | 0.67 | 1.66 | 11 | 3 |
| 1:A:4:VAL:HG23 | 1:A:202:ALA:HB3 | 0.67 | 1.66 | 3 | 3 |
| 1:A:69:TYR:CD2 | 1:A:70:THR:N | 0.67 | 2.62 | 1 | 3 |
| 1:A:147:LEU:HD13 | 1:A:251:ILE:HG12 | 0.67 | 1.67 | 7 | 5 |
| 1:A:60:ASN:CB | 1:A:97:TRP:CG | 0.66 | 2.78 | 9 | 11 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:100:ILE:HG12 | 1:A:115:ALA:HB1 | 0.66 | 1.66 | 2 | 16 |
| 1:A:139:GLY:H | 1:A:142:ARG:NH1 | 0.66 | 1.89 | 16 | 1 |
| 1:A:50:THR:HG23 | 1:A:120:MET:CE | 0.66 | 2.20 | 6 | 6 |
| 1:A:69:TYR:CE1 | 1:A:125:ILE:HG21 | 0.65 | 2.25 | 1 | 1 |
| 1:A:45:THR:O | 1:A:129:MET:HE3 | 0.65 | 1.91 | 14 | 10 |
| 1:A:160:ILE:HD12 | 1:A:170:TRP:CE3 | 0.65 | 2.26 | 6 | 1 |
| 1:A:60:ASN:CB | 1:A:97:TRP:CD2 | 0.65 | 2.80 | 1 | 12 |
| 1:A:178:LEU:HD21 | 1:A:199:ILE:HG22 | 0.65 | 1.67 | 7 | 2 |
| 1:A:38:PHE:CE2 | 1:A:133:PRO:CG | 0.65 | 2.80 | 4 | 3 |
| 1:A:138:ALA:HB2 | 1:A:142:ARG:NH2 | 0.65 | 2.07 | 10 | 2 |
| 1:A:93:ARG:HE | 1:A:118:GLU:HG2 | 0.64 | 1.52 | 7 | 6 |
| 1:A:197:PHE:CD1 | 1:A:212:TRP:CZ3 | 0.64 | 2.85 | 9 | 2 |
| 1:A:160:ILE:CD1 | 1:A:170:TRP:CZ3 | 0.64 | 2.81 | 6 | 3 |
| 1:A:19:ASN:CB | 1:A:20:PRO:CD | 0.64 | 2.76 | 4 | 20 |
| 1:A:59:HIS:CD2 | 1:A:251:ILE:O | 0.64 | 2.50 | 12 | 20 |
| 1:A:210:VAL:CG1 | 1:A:212:TRP:CE2 | 0.64 | 2.81 | 4 | 2 |
| 1:A:176:LYS:HZ3 | 1:A:176:LYS:HB3 | 0.64 | 1.52 | 5 | 1 |
| 1:A:86:LEU:HD12 | 1:A:86:LEU:N | 0.64 | 2.08 | 8 | 10 |
| 1:A:158:HIS:CE1 | 1:A:249:VAL:CG2 | 0.64 | 2.81 | 15 | 8 |
| 1:A:28:ILE:HD11 | 1:A:133:PRO:N | 0.64 | 2.08 | 17 | 17 |
| 1:A:7:LEU:HB3 | 1:A:58:TYR:CE2 | 0.64 | 2.28 | 5 | 18 |
| 1:A:90:ILE:HD12 | 1:A:150:ASN:OD1 | 0.64 | 1.93 | 1 | 1 |
| 1:A:186:TYR:CD1 | 1:A:197:PHE:CE2 | 0.64 | 2.86 | 11 | 6 |
| 1:A:174:ILE:HG21 | 1:A:199:ILE:CD1 | 0.63 | 2.23 | 12 | 6 |
| 1:A:38:PHE:CD2 | 1:A:79:TYR:CE1 | 0.63 | 2.86 | 13 | 3 |
| 1:A:137:SER:OG | 1:A:138:ALA:N | 0.63 | 2.31 | 17 | 20 |
| 1:A:185:TYR:CD1 | 1:A:248:VAL:CG2 | 0.63 | 2.81 | 18 | 11 |
| 1:A:162:ARG:N | 1:A:170:TRP:CH2 | 0.63 | 2.66 | 14 | 16 |
| 1:A:69:TYR:CD1 | 1:A:70:THR:N | 0.63 | 2.67 | 2 | 8 |
| 1:A:139:GLY:N | 1:A:142:ARG:NH1 | 0.63 | 2.47 | 16 | 1 |
| 1:A:21:TYR:HD1 | 1:A:120:MET:SD | 0.63 | 2.17 | 2 | 1 |
| 1:A:90:ILE:HG21 | 1:A:150:ASN:OD1 | 0.63 | 1.92 | 1 | 1 |
| 1:A:116:ILE:HD12 | 1:A:119:LEU:HD23 | 0.63 | 1.70 | 12 | 7 |
| 1:A:107:ARG:HE | 1:A:108:GLU:HA | 0.62 | 1.54 | 17 | 2 |
| 1:A:86:LEU:N | 1:A:86:LEU:HD12 | 0.62 | 2.09 | 7 | 7 |
| 1:A:160:ILE:CD1 | 1:A:170:TRP:CH2 | 0.62 | 2.80 | 9 | 5 |
| 1:A:80:PHE:CD1 | 1:A:80:PHE:N | 0.62 | 2.67 | 13 | 5 |
| 1:A:104:TYR:CE2 | 1:A:116:ILE:HG21 | 0.62 | 2.30 | 6 | 7 |
| 1:A:71:TYR:CE1 | 1:A:86:LEU:HB2 | 0.62 | 2.29 | 20 | 19 |
| 1:A:177:GLU:CG | 1:A:249:VAL:HB | 0.61 | 2.24 | 6 | 20 |
| 1:A:53:ALA:CB | 1:A:120:MET:SD | 0.61 | 2.89 | 20 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:27:VAL:HG23 | 1:A:42:HIS:CE1 | 0.61 | 2.30 | 19 | 1 |
| 1:A:38:PHE:CG | 1:A:133:PRO:HG3 | 0.61 | 2.31 | 16 | 20 |
| 1:A:139:GLY:H | 1:A:142:ARG:CZ | 0.61 | 2.08 | 16 | 1 |
| 1:A:200:ASP:OD1 | 1:A:209:HIS:CG | 0.61 | 2.54 | 19 | 6 |
| 1:A:139:GLY:O | 1:A:142:ARG:NH1 | 0.61 | 2.33 | 16 | 1 |
| 1:A:4:VAL:HG21 | 1:A:178:LEU:CB | 0.61 | 2.25 | 4 | 4 |
| 1:A:156:SER:O | 1:A:158:HIS:CE1 | 0.61 | 2.54 | 16 | 8 |
| 1:A:139:GLY:C | 1:A:142:ARG:HH12 | 0.61 | 1.99 | 16 | 1 |
| 1:A:81:ASN:O | 1:A:82:HIS:CG | 0.60 | 2.53 | 12 | 20 |
| 1:A:116:ILE:CD1 | 1:A:120:MET:HE2 | 0.60 | 2.20 | 18 | 1 |
| 1:A:69:TYR:CD1 | 1:A:125:ILE:CG2 | 0.60 | 2.84 | 1 | 1 |
| 1:A:158:HIS:NE2 | 1:A:249:VAL:CG2 | 0.60 | 2.64 | 14 | 18 |
| 1:A:15:TYR:CD2 | 1:A:54:GLN:CG | 0.60 | 2.85 | 19 | 7 |
| 1:A:158:HIS:CD2 | 1:A:249:VAL:CG2 | 0.60 | 2.84 | 18 | 10 |
| 1:A:209:HIS:C | 1:A:209:HIS:CD2 | 0.60 | 2.75 | 14 | 4 |
| 1:A:7:LEU:HB3 | 1:A:58:TYR:CE1 | 0.60 | 2.31 | 17 | 2 |
| 1:A:187:GLN:CA | 1:A:195:HIS:O | 0.60 | 2.50 | 19 | 17 |
| 1:A:184:VAL:CG1 | 1:A:249:VAL:HG12 | 0.60 | 2.26 | 8 | 3 |
| 1:A:142:ARG:NH1 | 1:A:142:ARG:HG3 | 0.60 | 2.12 | 16 | 1 |
| 1:A:200:ASP:OD2 | 1:A:209:HIS:CD2 | 0.60 | 2.55 | 7 | 8 |
| 1:A:90:ILE:HA | 1:A:93:ARG:CG | 0.59 | 2.28 | 1 | 20 |
| 1:A:189:VAL:CG1 | 1:A:190:GLY:N | 0.59 | 2.65 | 8 | 6 |
| 1:A:77:ASN:O | 1:A:82:HIS:CE1 | 0.59 | 2.55 | 20 | 19 |
| 1:A:187:GLN:HA | 1:A:195:HIS:O | 0.59 | 1.97 | 10 | 20 |
| 1:A:28:ILE:HG23 | 1:A:79:TYR:HB3 | 0.59 | 1.73 | 20 | 3 |
| 1:A:137:SER:OG | 1:A:142:ARG:NE | 0.59 | 2.34 | 16 | 1 |
| 1:A:162:ARG:CD | 1:A:170:TRP:CG | 0.59 | 2.85 | 4 | 3 |
| 1:A:6:SER:OG | 1:A:209:HIS:CG | 0.59 | 2.56 | 2 | 4 |
| 1:A:93:ARG:NE | 1:A:118:GLU:CG | 0.59 | 2.66 | 11 | 12 |
| 1:A:127:VAL:HB | 1:A:142:ARG:NE | 0.59 | 2.12 | 16 | 1 |
| 1:A:26:PRO:HG2 | 1:A:131:TYR:CG | 0.59 | 2.31 | 6 | 16 |
| 1:A:90:ILE:CG2 | 1:A:150:ASN:OD1 | 0.59 | 2.50 | 1 | 1 |
| 1:A:90:ILE:CD1 | 1:A:150:ASN:OD1 | 0.59 | 2.51 | 1 | 1 |
| 1:A:209:HIS:CD2 | 1:A:210:VAL:N | 0.59 | 2.71 | 14 | 5 |
| 1:A:209:HIS:CD2 | 1:A:209:HIS:C | 0.59 | 2.76 | 11 | 3 |
| 1:A:60:ASN:OD1 | 1:A:97:TRP:CE3 | 0.59 | 2.55 | 15 | 10 |
| 1:A:7:LEU:HD13 | 1:A:181:ASN:C | 0.59 | 2.18 | 19 | 13 |
| 1:A:142:ARG:CB | 1:A:142:ARG:CZ | 0.59 | 2.77 | 16 | 1 |
| 1:A:186:TYR:HB3 | 1:A:197:PHE:CE1 | 0.58 | 2.33 | 3 | 16 |
| 1:A:97:TRP:CE3 | 1:A:100:ILE:HD12 | 0.58 | 2.33 | 2 | 14 |
| 1:A:170:TRP:HE1 | 1:A:174:ILE:HD11 | 0.58 | 1.56 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:199:ILE:HG23 | 1:A:208:TYR:HB3 | 0.58 | 1.74 | 1 | 2 |
| 1:A:19:ASN:ND2 | 1:A:20:PRO:HD3 | 0.58 | 2.14 | 19 | 16 |
| 1:A:202:ALA:HB1 | 1:A:208:TYR:CE1 | 0.58 | 2.33 | 13 | 1 |
| 1:A:28:ILE:HD11 | 1:A:132:GLY:HA2 | 0.58 | 1.76 | 16 | 3 |
| 1:A:60:ASN:HB2 | 1:A:97:TRP:CG | 0.58 | 2.33 | 17 | 9 |
| 1:A:186:TYR:HB3 | 1:A:197:PHE:CZ | 0.58 | 2.34 | 12 | 19 |
| 1:A:158:HIS:CE1 | 1:A:249:VAL:O | 0.58 | 2.56 | 20 | 6 |
| 1:A:7:LEU:N | 1:A:200:ASP:O | 0.58 | 2.36 | 18 | 16 |
| 1:A:158:HIS:CD2 | 1:A:249:VAL:HG23 | 0.58 | 2.33 | 18 | 5 |
| 1:A:162:ARG:HB2 | 1:A:170:TRP:CZ2 | 0.58 | 2.34 | 3 | 17 |
| 1:A:139:GLY:HA2 | 1:A:185:TYR:OH | 0.58 | 1.99 | 18 | 19 |
| 1:A:174:ILE:CG2 | 1:A:199:ILE:HG21 | 0.58 | 2.28 | 7 | 5 |
| 1:A:21:TYR:CD1 | 1:A:120:MET:SD | 0.58 | 2.96 | 2 | 1 |
| 1:A:69:TYR:OH | 1:A:71:TYR:CD2 | 0.58 | 2.54 | 1 | 1 |
| 1:A:61:TYR:CD1 | 1:A:61:TYR:C | 0.58 | 2.77 | 3 | 12 |
| 1:A:200:ASP:OD1 | 1:A:209:HIS:CD2 | 0.58 | 2.57 | 11 | 8 |
| 1:A:162:ARG:CG | 1:A:245:GLN:NE2 | 0.58 | 2.67 | 13 | 2 |
| 1:A:38:PHE:CD1 | 1:A:41:GLN:NE2 | 0.58 | 2.72 | 13 | 3 |
| 1:A:142:ARG:CG | 1:A:142:ARG:NH1 | 0.58 | 2.65 | 16 | 1 |
| 1:A:19:ASN:CG | 1:A:20:PRO:CD | 0.58 | 2.72 | 18 | 16 |
| 1:A:15:TYR:CG | 1:A:54:GLN:HG2 | 0.58 | 2.34 | 19 | 5 |
| 1:A:48:VAL:HA | 1:A:196:ALA:CB | 0.58 | 2.29 | 13 | 16 |
| 1:A:153:TYR:CD2 | 1:A:251:ILE:HG22 | 0.57 | 2.34 | 19 | 6 |
| 1:A:101:LEU:N | 1:A:104:TYR:OH | 0.57 | 2.37 | 3 | 16 |
| 1:A:6:SER:OG | 1:A:209:HIS:CD2 | 0.57 | 2.56 | 15 | 3 |
| 1:A:26:PRO:HG3 | 1:A:86:LEU:HD21 | 0.57 | 1.76 | 16 | 3 |
| 1:A:186:TYR:CD1 | 1:A:187:GLN:N | 0.57 | 2.72 | 4 | 15 |
| 1:A:210:VAL:HG11 | 1:A:212:TRP:CH2 | 0.57 | 2.34 | 6 | 1 |
| 1:A:178:LEU:HD11 | 1:A:199:ILE:CG2 | 0.57 | 2.28 | 17 | 5 |
| 1:A:185:TYR:CD1 | 1:A:185:TYR:C | 0.57 | 2.77 | 13 | 7 |
| 1:A:93:ARG:HE | 1:A:118:GLU:CG | 0.57 | 2.11 | 8 | 9 |
| 1:A:160:ILE:HD11 | 1:A:247:ALA:HB3 | 0.57 | 1.74 | 17 | 9 |
| 1:A:69:TYR:CZ | 1:A:125:ILE:CG2 | 0.57 | 2.82 | 1 | 1 |
| 1:A:52:THR:HG23 | 1:A:147:LEU:HD21 | 0.57 | 1.77 | 2 | 1 |
| 1:A:59:HIS:NE2 | 1:A:251:ILE:O | 0.57 | 2.37 | 3 | 14 |
| 1:A:71:TYR:OH | 1:A:86:LEU:HD22 | 0.57 | 1.99 | 6 | 10 |
| 1:A:139:GLY:CA | 1:A:185:TYR:OH | 0.57 | 2.52 | 17 | 17 |
| 1:A:19:ASN:CB | 1:A:20:PRO:HD3 | 0.57 | 2.30 | 18 | 3 |
| 1:A:19:ASN:HB2 | 1:A:20:PRO:HD3 | 0.57 | 1.75 | 18 | 1 |
| 1:A:4:VAL:HB | 1:A:202:ALA:N | 0.56 | 2.14 | 1 | 14 |
| 1:A:60:ASN:HB3 | 1:A:97:TRP:CD2 | 0.56 | 2.34 | 8 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:45:THR:O | 1:A:129:MET:CE | 0.56 | 2.53 | 14 | 14 |
| 1:A:200:ASP:N | 1:A:200:ASP:OD1 | 0.56 | 2.38 | 17 | 1 |
| 1:A:60:ASN:HA | 1:A:97:TRP:CD2 | 0.56 | 2.35 | 14 | 20 |
| 1:A:60:ASN:HA | 1:A:97:TRP:CE2 | 0.56 | 2.35 | 1 | 18 |
| 1:A:80:PHE:N | 1:A:80:PHE:CD1 | 0.56 | 2.74 | 11 | 3 |
| 1:A:15:TYR:CD2 | 1:A:54:GLN:HG2 | 0.56 | 2.35 | 19 | 8 |
| 1:A:90:ILE:CB | 1:A:150:ASN:OD1 | 0.56 | 2.53 | 1 | 1 |
| 1:A:154:ASN:CB | 1:A:252:LYS:O | 0.56 | 2.54 | 12 | 20 |
| 1:A:208:TYR:N | 1:A:208:TYR:CD1 | 0.56 | 2.74 | 7 | 5 |
| 1:A:69:TYR:CD1 | 1:A:150:ASN:OD1 | 0.56 | 2.58 | 13 | 1 |
| 1:A:57:LYS:CE | 1:A:100:ILE:O | 0.56 | 2.54 | 17 | 16 |
| 1:A:15:TYR:HB2 | 1:A:54:GLN:CG | 0.56 | 2.30 | 14 | 20 |
| 1:A:13:ILE:HD11 | 1:A:58:TYR:HA | 0.56 | 1.78 | 20 | 10 |
| 1:A:52:THR:O | 1:A:56:MET:N | 0.56 | 2.38 | 3 | 10 |
| 1:A:128:ASP:HB2 | 1:A:142:ARG:HE | 0.56 | 1.59 | 17 | 2 |
| 1:A:170:TRP:NE1 | 1:A:186:TYR:OH | 0.56 | 2.39 | 1 | 17 |
| 1:A:62:PRO:O | 1:A:95:TYR:HB2 | 0.56 | 2.00 | 15 | 18 |
| 1:A:160:ILE:O | 1:A:246:SER:CB | 0.55 | 2.55 | 12 | 15 |
| 1:A:85:ASN:N | 1:A:85:ASN:ND2 | 0.55 | 2.54 | 13 | 5 |
| 1:A:185:TYR:C | 1:A:185:TYR:CD1 | 0.55 | 2.79 | 7 | 12 |
| 1:A:205:ARG:O | 1:A:206:ASN:CB | 0.55 | 2.55 | 5 | 8 |
| 1:A:30:LYS:N | 1:A:79:TYR:O | 0.55 | 2.40 | 19 | 14 |
| 1:A:67:LYS:O | 1:A:150:ASN:OD1 | 0.55 | 2.23 | 1 | 1 |
| 1:A:61:TYR:CD1 | 1:A:253:PRO:HB3 | 0.55 | 2.36 | 12 | 20 |
| 1:A:199:ILE:HA | 1:A:209:HIS:O | 0.55 | 2.01 | 17 | 2 |
| 1:A:126:SER:OG | 1:A:146:ALA:HB1 | 0.55 | 2.01 | 1 | 3 |
| 1:A:200:ASP:CG | 1:A:209:HIS:CD2 | 0.55 | 2.80 | 10 | 8 |
| 1:A:162:ARG:N | 1:A:170:TRP:CZ3 | 0.55 | 2.74 | 20 | 8 |
| 1:A:162:ARG:HD3 | 1:A:170:TRP:CD1 | 0.55 | 2.37 | 14 | 11 |
| 1:A:73:LEU:HD21 | 1:A:80:PHE:CD1 | 0.55 | 2.37 | 13 | 1 |
| 1:A:61:TYR:CB | 1:A:62:PRO:CD | 0.55 | 2.85 | 7 | 20 |
| 1:A:100:ILE:CG1 | 1:A:115:ALA:HB1 | 0.55 | 2.31 | 2 | 10 |
| 1:A:78:PRO:HD2 | 1:A:79:TYR:CD2 | 0.55 | 2.37 | 17 | 20 |
| 1:A:162:ARG:HD2 | 1:A:170:TRP:CG | 0.55 | 2.37 | 4 | 6 |
| 1:A:38:PHE:CE2 | 1:A:79:TYR:CE1 | 0.55 | 2.95 | 13 | 3 |
| 1:A:54:GLN:OE1 | 1:A:211:ASN:ND2 | 0.55 | 2.40 | 14 | 15 |
| 1:A:174:ILE:CG2 | 1:A:184:VAL:HG21 | 0.55 | 2.25 | 11 | 4 |
| 1:A:184:VAL:HB | 1:A:199:ILE:HB | 0.55 | 1.77 | 10 | 5 |
| 1:A:60:ASN:HB3 | 1:A:97:TRP:CG | 0.55 | 2.37 | 16 | 15 |
| 1:A:4:VAL:HG12 | 1:A:201:GLY:HA2 | 0.55 | 1.78 | 17 | 1 |
| 1:A:25:THR:O | 1:A:42:HIS:CE1 | 0.55 | 2.60 | 17 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:8:LEU:HD11 | 1:A:198:VAL:HG11 | 0.55 | 1.77 | 2 | 5 |
| 1:A:17:GLN:CG | 1:A:50:THR:OG1 | 0.55 | 2.55 | 20 | 1 |
| 1:A:60:ASN:HA | 1:A:97:TRP:CE3 | 0.54 | 2.37 | 12 | 7 |
| 1:A:208:TYR:CD1 | 1:A:208:TYR:N | 0.54 | 2.74 | 6 | 6 |
| 1:A:61:TYR:HB3 | 1:A:62:PRO:HD3 | 0.54 | 1.80 | 13 | 20 |
| 1:A:38:PHE:CE2 | 1:A:133:PRO:HG2 | 0.54 | 2.37 | 13 | 3 |
| 1:A:6:SER:HB3 | 1:A:209:HIS:CD2 | 0.54 | 2.37 | 17 | 1 |
| 1:A:15:TYR:OH | 1:A:57:LYS:HB2 | 0.54 | 2.03 | 4 | 20 |
| 1:A:189:VAL:HG12 | 1:A:190:GLY:N | 0.54 | 2.17 | 9 | 17 |
| 1:A:69:TYR:CD1 | 1:A:69:TYR:O | 0.54 | 2.60 | 1 | 1 |
| 1:A:19:ASN:CB | 1:A:20:PRO:HD2 | 0.54 | 2.33 | 19 | 9 |
| 1:A:79:TYR:C | 1:A:80:PHE:CD1 | 0.54 | 2.81 | 8 | 5 |
| 1:A:14:HIS:N | 1:A:102:PRO:O | 0.54 | 2.39 | 15 | 20 |
| 1:A:28:ILE:CD1 | 1:A:133:PRO:HD3 | 0.54 | 2.33 | 13 | 20 |
| 1:A:60:ASN:HB3 | 1:A:97:TRP:CE3 | 0.54 | 2.38 | 12 | 4 |
| 1:A:19:ASN:N | 1:A:19:ASN:ND2 | 0.54 | 2.52 | 18 | 1 |
| 1:A:156:SER:O | 1:A:158:HIS:ND1 | 0.54 | 2.41 | 11 | 16 |
| 1:A:4:VAL:CG1 | 1:A:201:GLY:HA2 | 0.54 | 2.33 | 17 | 3 |
| 1:A:38:PHE:CG | 1:A:41:GLN:NE2 | 0.54 | 2.76 | 13 | 3 |
| 1:A:93:ARG:CD | 1:A:122:ASP:OD2 | 0.54 | 2.56 | 9 | 3 |
| 1:A:177:GLU:HG3 | 1:A:249:VAL:HB | 0.54 | 1.80 | 6 | 6 |
| 1:A:203:ASP:N | 1:A:207:PHE:O | 0.54 | 2.41 | 12 | 6 |
| 1:A:65:GLY:C | 1:A:66:LEU:HD23 | 0.54 | 2.23 | 15 | 1 |
| 1:A:174:ILE:HG21 | 1:A:199:ILE:HG21 | 0.54 | 1.79 | 16 | 3 |
| 1:A:59:HIS:O | 1:A:60:ASN:C | 0.54 | 2.46 | 8 | 20 |
| 1:A:185:TYR:HB3 | 1:A:248:VAL:HB | 0.54 | 1.79 | 17 | 9 |
| 1:A:186:TYR:HB3 | 1:A:197:PHE:CE2 | 0.53 | 2.38 | 1 | 1 |
| 1:A:60:ASN:CA | 1:A:97:TRP:CD2 | 0.53 | 2.91 | 1 | 14 |
| 1:A:107:ARG:O | 1:A:107:ARG:CD | 0.53 | 2.57 | 8 | 3 |
| 1:A:16:ASN:HB2 | 1:A:21:TYR:CE1 | 0.53 | 2.39 | 6 | 2 |
| 1:A:65:GLY:HA3 | 1:A:90:ILE:O | 0.53 | 2.04 | 3 | 20 |
| 1:A:60:ASN:CA | 1:A:97:TRP:CE2 | 0.53 | 2.91 | 1 | 15 |
| 1:A:29:GLU:HA | 1:A:39:VAL:HG13 | 0.53 | 1.80 | 1 | 5 |
| 1:A:15:TYR:OH | 1:A:57:LYS:CG | 0.53 | 2.57 | 18 | 2 |
| 1:A:160:ILE:O | 1:A:246:SER:CA | 0.53 | 2.56 | 12 | 17 |
| 1:A:19:ASN:CG | 1:A:20:PRO:HD3 | 0.53 | 2.23 | 7 | 20 |
| 1:A:187:GLN:HG3 | 1:A:187:GLN:O | 0.53 | 2.03 | 1 | 9 |
| 1:A:200:ASP:OD1 | 1:A:209:HIS:ND1 | 0.53 | 2.42 | 1 | 3 |
| 1:A:21:TYR:CD2 | 1:A:116:ILE:HG12 | 0.53 | 2.38 | 3 | 7 |
| 1:A:139:GLY:CA | 1:A:187:GLN:OE1 | 0.53 | 2.56 | 3 | 2 |
| 1:A:177:GLU:OE1 | 1:A:182:GLN:CB | 0.53 | 2.57 | 18 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:124:GLY:O | 1:A:129:MET:CB | 0.53 | 2.57 | 6 | 10 |
| 1:A:139:GLY:O | 1:A:143:VAL:HG23 | 0.53 | 2.03 | 7 | 3 |
| 1:A:69:TYR:CD1 | 1:A:125:ILE:HG21 | 0.53 | 2.39 | 1 | 1 |
| 1:A:16:ASN:HB2 | 1:A:21:TYR:CE2 | 0.53 | 2.39 | 20 | 4 |
| 1:A:170:TRP:CZ2 | 1:A:186:TYR:CE2 | 0.53 | 2.96 | 3 | 16 |
| 1:A:160:ILE:N | 1:A:247:ALA:O | 0.53 | 2.40 | 9 | 9 |
| 1:A:143:VAL:HG12 | 1:A:147:LEU:CD1 | 0.53 | 2.34 | 15 | 13 |
| 1:A:57:LYS:O | 1:A:60:ASN:ND2 | 0.53 | 2.42 | 1 | 9 |
| 1:A:180:GLN:O | 1:A:182:GLN:CG | 0.53 | 2.57 | 13 | 2 |
| 1:A:38:PHE:CD2 | 1:A:133:PRO:CD | 0.53 | 2.92 | 4 | 3 |
| 1:A:183:PRO:CB | 1:A:199:ILE:O | 0.53 | 2.57 | 17 | 1 |
| 1:A:44:ALA:CB | 1:A:135:SER:OG | 0.53 | 2.57 | 4 | 1 |
| 1:A:120:MET:O | 1:A:124:GLY:N | 0.53 | 2.38 | 14 | 16 |
| 1:A:178:LEU:HD13 | 1:A:201:GLY:O | 0.53 | 2.03 | 5 | 8 |
| 1:A:116:ILE:HG23 | 1:A:117:SER:N | 0.53 | 2.19 | 18 | 4 |
| 1:A:93:ARG:CD | 1:A:118:GLU:OE1 | 0.53 | 2.57 | 14 | 1 |
| 1:A:85:ASN:ND2 | 1:A:85:ASN:N | 0.53 | 2.57 | 17 | 1 |
| 1:A:176:LYS:CB | 1:A:176:LYS:NZ | 0.53 | 2.70 | 5 | 1 |
| 1:A:68:ASP:N | 1:A:91:SER:OG | 0.53 | 2.42 | 6 | 2 |
| 1:A:62:PRO:O | 1:A:95:TYR:CB | 0.53 | 2.57 | 11 | 12 |
| 1:A:162:ARG:N | 1:A:245:GLN:O | 0.53 | 2.42 | 14 | 5 |
| 1:A:61:TYR:C | 1:A:61:TYR:CD1 | 0.52 | 2.81 | 8 | 8 |
| 1:A:143:VAL:HG21 | 1:A:185:TYR:CZ | 0.52 | 2.39 | 14 | 5 |
| 1:A:202:ALA:HB2 | 1:A:208:TYR:CE1 | 0.52 | 2.39 | 13 | 1 |
| 1:A:48:VAL:HA | 1:A:196:ALA:HB3 | 0.52 | 1.80 | 17 | 14 |
| 1:A:130:ASP:CB | 1:A:136:GLY:O | 0.52 | 2.57 | 15 | 8 |
| 1:A:56:MET:O | 1:A:60:ASN:N | 0.52 | 2.42 | 10 | 8 |
| 1:A:145:ARG:CG | 1:A:149:GLU:OE1 | 0.52 | 2.58 | 17 | 2 |
| 1:A:162:ARG:HD2 | 1:A:170:TRP:CD2 | 0.52 | 2.38 | 4 | 6 |
| 1:A:185:TYR:O | 1:A:185:TYR:CD1 | 0.52 | 2.62 | 9 | 10 |
| 1:A:175:ASP:O | 1:A:179:SER:N | 0.52 | 2.41 | 14 | 13 |
| 1:A:17:GLN:OE1 | 1:A:47:SER:N | 0.52 | 2.42 | 18 | 2 |
| 1:A:15:TYR:OH | 1:A:57:LYS:CB | 0.52 | 2.57 | 2 | 4 |
| 1:A:68:ASP:OD1 | 1:A:91:SER:N | 0.52 | 2.43 | 14 | 5 |
| 1:A:69:TYR:C | 1:A:69:TYR:CD1 | 0.52 | 2.83 | 2 | 1 |
| 1:A:93:ARG:NE | 1:A:118:GLU:HG2 | 0.52 | 2.19 | 20 | 9 |
| 1:A:44:ALA:N | 1:A:135:SER:OG | 0.52 | 2.43 | 18 | 9 |
| 1:A:197:PHE:HB3 | 1:A:212:TRP:CE3 | 0.52 | 2.40 | 19 | 1 |
| 1:A:8:LEU:HD12 | 1:A:211:ASN:CB | 0.52 | 2.34 | 17 | 1 |
| 1:A:171:GLU:CG | 1:A:208:TYR:OH | 0.52 | 2.58 | 16 | 1 |
| 1:A:82:HIS:N | 1:A:83:PRO:HD2 | 0.52 | 2.20 | 18 | 20 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:7:LEU:HB2 | 1:A:200:ASP:HB2 | 0.52 | 1.81 | 3 | 19 |
| 1:A:56:MET:SD | 1:A:123:VAL:CG2 | 0.52 | 2.98 | 20 | 3 |
| 1:A:199:ILE:HG12 | 1:A:210:VAL:HG22 | 0.52 | 1.82 | 16 | 2 |
| 1:A:71:TYR:CB | 1:A:128:ASP:OD1 | 0.52 | 2.58 | 15 | 5 |
| 1:A:153:TYR:CE2 | 1:A:251:ILE:HG22 | 0.52 | 2.40 | 19 | 3 |
| 1:A:178:LEU:CD1 | 1:A:201:GLY:O | 0.52 | 2.58 | 1 | 3 |
| 1:A:11:LYS:HG3 | 1:A:58:TYR:CE1 | 0.52 | 2.40 | 17 | 1 |
| 1:A:104:TYR:CE2 | 1:A:116:ILE:CG2 | 0.52 | 2.93 | 6 | 5 |
| 1:A:5:LYS:O | 1:A:200:ASP:O | 0.52 | 2.28 | 19 | 15 |
| 1:A:56:MET:SD | 1:A:123:VAL:HG22 | 0.52 | 2.45 | 5 | 8 |
| 1:A:160:ILE:O | 1:A:247:ALA:N | 0.52 | 2.42 | 15 | 7 |
| 1:A:107:ARG:O | 1:A:107:ARG:NE | 0.52 | 2.42 | 17 | 3 |
| 1:A:57:LYS:NZ | 1:A:100:ILE:O | 0.52 | 2.43 | 17 | 7 |
| 1:A:184:VAL:HG22 | 1:A:249:VAL:HG12 | 0.52 | 1.82 | 18 | 2 |
| 1:A:107:ARG:HE | 1:A:108:GLU:CA | 0.52 | 2.18 | 17 | 1 |
| 1:A:210:VAL:HG11 | 1:A:212:TRP:CE3 | 0.51 | 2.40 | 6 | 1 |
| 1:A:162:ARG:HA | 1:A:170:TRP:CE3 | 0.51 | 2.40 | 4 | 12 |
| 1:A:93:ARG:NE | 1:A:122:ASP:OD2 | 0.51 | 2.42 | 6 | 4 |
| 1:A:67:LYS:O | 1:A:150:ASN:ND2 | 0.51 | 2.43 | 1 | 2 |
| 1:A:175:ASP:N | 1:A:175:ASP:OD1 | 0.51 | 2.43 | 17 | 1 |
| 1:A:82:HIS:N | 1:A:83:PRO:CD | 0.51 | 2.73 | 18 | 20 |
| 1:A:90:ILE:O | 1:A:93:ARG:N | 0.51 | 2.43 | 14 | 14 |
| 1:A:160:ILE:CG1 | 1:A:247:ALA:HB3 | 0.51 | 2.35 | 8 | 9 |
| 1:A:107:ARG:CD | 1:A:107:ARG:O | 0.51 | 2.58 | 19 | 1 |
| 1:A:24:LEU:HD13 | 1:A:118:GLU:OE1 | 0.51 | 2.05 | 20 | 1 |
| 1:A:176:LYS:CB | 1:A:176:LYS:HZ3 | 0.51 | 2.19 | 5 | 1 |
| 1:A:49:ALA:HB2 | 1:A:129:MET:HE3 | 0.51 | 1.82 | 19 | 4 |
| 1:A:145:ARG:NE | 1:A:149:GLU:OE2 | 0.51 | 2.44 | 5 | 1 |
| 1:A:162:ARG:HB2 | 1:A:170:TRP:CE2 | 0.51 | 2.41 | 14 | 17 |
| 1:A:28:ILE:HD13 | 1:A:133:PRO:HD3 | 0.51 | 1.82 | 10 | 19 |
| 1:A:187:GLN:CB | 1:A:195:HIS:O | 0.51 | 2.58 | 13 | 14 |
| 1:A:26:PRO:HD2 | 1:A:131:TYR:CD1 | 0.51 | 2.40 | 3 | 10 |
| 1:A:15:TYR:HA | 1:A:21:TYR:CE1 | 0.51 | 2.41 | 2 | 2 |
| 1:A:55:ILE:CD1 | 1:A:198:VAL:CG2 | 0.51 | 2.84 | 2 | 2 |
| 1:A:186:TYR:CB | 1:A:197:PHE:CZ | 0.51 | 2.93 | 4 | 10 |
| 1:A:26:PRO:HG3 | 1:A:86:LEU:CD2 | 0.51 | 2.34 | 1 | 20 |
| 1:A:166:SER:O | 1:A:167:LYS:C | 0.51 | 2.49 | 7 | 20 |
| 1:A:13:ILE:O | 1:A:14:HIS:ND1 | 0.51 | 2.43 | 8 | 3 |
| 1:A:61:TYR:HB3 | 1:A:62:PRO:CD | 0.51 | 2.36 | 13 | 20 |
| 1:A:11:LYS:HG3 | 1:A:58:TYR:CE2 | 0.51 | 2.41 | 12 | 5 |
| 1:A:96:ASN:OD1 | 1:A:99:ASN:N | 0.51 | 2.43 | 12 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:178:LEU:HD13 | 1:A:201:GLY:C | 0.51 | 2.26 | 13 | 1 |
| 1:A:44:ALA:O | 1:A:135:SER:OG | 0.51 | 2.26 | 1 | 20 |
| 1:A:185:TYR:HD1 | 1:A:248:VAL:HG23 | 0.51 | 1.63 | 12 | 6 |
| 1:A:210:VAL:HG11 | 1:A:212:TRP:CD2 | 0.51 | 2.40 | 4 | 2 |
| 1:A:90:ILE:HB | 1:A:150:ASN:OD1 | 0.51 | 2.06 | 1 | 1 |
| 1:A:171:GLU:CB | 1:A:208:TYR:OH | 0.51 | 2.59 | 16 | 1 |
| 1:A:138:ALA:HB2 | 1:A:142:ARG:HH21 | 0.51 | 1.66 | 1 | 1 |
| 1:A:93:ARG:NH2 | 1:A:122:ASP:OD1 | 0.51 | 2.43 | 8 | 1 |
| 1:A:79:TYR:CZ | 1:A:133:PRO:HD2 | 0.50 | 2.41 | 1 | 7 |
| 1:A:63:ASN:O | 1:A:95:TYR:N | 0.50 | 2.44 | 1 | 8 |
| 1:A:145:ARG:CG | 1:A:149:GLU:OE2 | 0.50 | 2.59 | 6 | 2 |
| 1:A:68:ASP:HB3 | 1:A:87:PHE:CE1 | 0.50 | 2.41 | 16 | 6 |
| 1:A:17:GLN:NE2 | 1:A:47:SER:N | 0.50 | 2.59 | 13 | 1 |
| 1:A:69:TYR:OH | 1:A:86:LEU:O | 0.50 | 2.30 | 1 | 1 |
| 1:A:64:LYS:CG | 1:A:93:ARG:O | 0.50 | 2.59 | 1 | 1 |
| 1:A:185:TYR:CD1 | 1:A:248:VAL:HB | 0.50 | 2.42 | 18 | 6 |
| 1:A:28:ILE:HB | 1:A:38:PHE:O | 0.50 | 2.06 | 19 | 15 |
| 1:A:78:PRO:HG2 | 1:A:79:TYR:CE2 | 0.50 | 2.41 | 17 | 3 |
| 1:A:160:ILE:HG13 | 1:A:170:TRP:CH2 | 0.50 | 2.41 | 1 | 6 |
| 1:A:127:VAL:HA | 1:A:142:ARG:HB3 | 0.50 | 1.83 | 20 | 18 |
| 1:A:140:SER:HB3 | 1:A:159:GLN:CG | 0.50 | 2.35 | 5 | 11 |
| 1:A:202:ALA:HA | 1:A:208:TYR:CD1 | 0.50 | 2.41 | 13 | 1 |
| 1:A:21:TYR:CB | 1:A:120:MET:SD | 0.50 | 2.99 | 2 | 1 |
| 1:A:187:GLN:OE1 | 1:A:194:GLY:HA3 | 0.50 | 2.06 | 15 | 17 |
| 1:A:140:SER:HG | 1:A:185:TYR:HE1 | 0.50 | 1.48 | 3 | 2 |
| 1:A:159:GLN:CG | 1:A:160:ILE:N | 0.50 | 2.74 | 20 | 2 |
| 1:A:107:ARG:CD | 1:A:107:ARG:C | 0.50 | 2.80 | 10 | 2 |
| 1:A:19:ASN:HB3 | 1:A:21:TYR:CE1 | 0.50 | 2.42 | 13 | 9 |
| 1:A:24:LEU:HD12 | 1:A:117:SER:OG | 0.50 | 2.06 | 7 | 2 |
| 1:A:4:VAL:O | 1:A:202:ALA:N | 0.50 | 2.41 | 2 | 3 |
| 1:A:72:THR:HG23 | 1:A:85:ASN:CG | 0.50 | 2.27 | 9 | 2 |
| 1:A:93:ARG:CD | 1:A:118:GLU:CD | 0.50 | 2.80 | 11 | 1 |
| 1:A:60:ASN:HA | 1:A:97:TRP:CZ3 | 0.50 | 2.42 | 12 | 3 |
| 1:A:171:GLU:O | 1:A:175:ASP:N | 0.50 | 2.44 | 7 | 3 |
| 1:A:101:LEU:HB2 | 1:A:104:TYR:CZ | 0.50 | 2.42 | 17 | 8 |
| 1:A:77:ASN:ND2 | 1:A:130:ASP:OD1 | 0.50 | 2.44 | 4 | 1 |
| 1:A:198:VAL:O | 1:A:210:VAL:HA | 0.49 | 2.07 | 2 | 6 |
| 1:A:20:PRO:CA | 1:A:23:LEU:HD12 | 0.49 | 2.36 | 6 | 3 |
| 1:A:93:ARG:NE | 1:A:122:ASP:OD1 | 0.49 | 2.45 | 8 | 7 |
| 1:A:140:SER:O | 1:A:144:GLN:N | 0.49 | 2.44 | 5 | 7 |
| 1:A:125:ILE:HG22 | 1:A:126:SER:N | 0.49 | 2.21 | 16 | 6 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:145:ARG:NH1 | 1:A:149:GLU:OE2 | 0.49 | 2.45 | 18 | 1 |
| 1:A:73:LEU:CD2 | 1:A:80:PHE:CD1 | 0.49 | 2.94 | 13 | 1 |
| 1:A:11:LYS:HD2 | 1:A:58:TYR:CE2 | 0.49 | 2.42 | 10 | 1 |
| 1:A:18:GLY:O | 1:A:22:ASN:OD1 | 0.49 | 2.30 | 10 | 20 |
| 1:A:93:ARG:NE | 1:A:122:ASP:CG | 0.49 | 2.66 | 6 | 4 |
| 1:A:6:SER:HB2 | 1:A:209:HIS:CD2 | 0.49 | 2.42 | 1 | 1 |
| 1:A:186:TYR:O | 1:A:196:ALA:HA | 0.49 | 2.06 | 3 | 6 |
| 1:A:61:TYR:CB | 1:A:62:PRO:HD3 | 0.49 | 2.36 | 13 | 13 |
| 1:A:200:ASP:OD1 | 1:A:200:ASP:N | 0.49 | 2.43 | 16 | 2 |
| 1:A:154:ASN:OD1 | 1:A:155:GLN:N | 0.49 | 2.45 | 9 | 3 |
| 1:A:21:TYR:CD2 | 1:A:116:ILE:CG1 | 0.49 | 2.95 | 4 | 10 |
| 1:A:6:SER:HB2 | 1:A:209:HIS:CG | 0.49 | 2.42 | 16 | 5 |
| 1:A:162:ARG:HB2 | 1:A:186:TYR:HH | 0.49 | 1.68 | 7 | 7 |
| 1:A:197:PHE:CB | 1:A:212:TRP:HA | 0.49 | 2.36 | 4 | 8 |
| 1:A:93:ARG:CZ | 1:A:118:GLU:OE2 | 0.49 | 2.60 | 17 | 2 |
| 1:A:11:LYS:CD | 1:A:58:TYR:CD1 | 0.49 | 2.95 | 17 | 1 |
| 1:A:68:ASP:O | 1:A:150:ASN:ND2 | 0.49 | 2.45 | 11 | 2 |
| 1:A:76:ASN:ND2 | 1:A:76:ASN:O | 0.49 | 2.44 | 11 | 1 |
| 1:A:129:MET:HB3 | 1:A:131:TYR:CZ | 0.49 | 2.42 | 9 | 6 |
| 1:A:7:LEU:HD22 | 1:A:181:ASN:HB3 | 0.49 | 1.83 | 18 | 2 |
| 1:A:175:ASP:OD1 | 1:A:175:ASP:N | 0.49 | 2.45 | 12 | 2 |
| 1:A:185:TYR:CD2 | 1:A:248:VAL:HG23 | 0.49 | 2.42 | 14 | 1 |
| 1:A:68:ASP:OD1 | 1:A:68:ASP:N | 0.49 | 2.46 | 17 | 2 |
| 1:A:177:GLU:CD | 1:A:250:GLY:N | 0.49 | 2.66 | 6 | 6 |
| 1:A:7:LEU:CD1 | 1:A:181:ASN:C | 0.49 | 2.81 | 19 | 8 |
| 1:A:160:ILE:CD1 | 1:A:247:ALA:HB3 | 0.49 | 2.38 | 19 | 9 |
| 1:A:139:GLY:HA3 | 1:A:187:GLN:OE1 | 0.49 | 2.08 | 18 | 19 |
| 1:A:69:TYR:CB | 1:A:150:ASN:ND2 | 0.49 | 2.75 | 1 | 1 |
| 1:A:205:ARG:O | 1:A:207:PHE:N | 0.49 | 2.46 | 1 | 1 |
| 1:A:139:GLY:C | 1:A:185:TYR:OH | 0.49 | 2.51 | 16 | 6 |
| 1:A:30:LYS:CD | 1:A:80:PHE:C | 0.49 | 2.81 | 12 | 2 |
| 1:A:154:ASN:ND2 | 1:A:156:SER:OG | 0.49 | 2.46 | 3 | 1 |
| 1:A:103:THR:HG23 | 1:A:103:THR:O | 0.49 | 2.07 | 20 | 3 |
| 1:A:177:GLU:HG3 | 1:A:184:VAL:HG22 | 0.49 | 1.85 | 6 | 1 |
| 1:A:93:ARG:NH1 | 1:A:118:GLU:OE2 | 0.49 | 2.46 | 6 | 1 |
| 1:A:148:LYS:CG | 1:A:157:VAL:HB | 0.49 | 2.38 | 19 | 13 |
| 1:A:19:ASN:HB3 | 1:A:21:TYR:CD2 | 0.49 | 2.43 | 1 | 1 |
| 1:A:61:TYR:CD2 | 1:A:62:PRO:HD3 | 0.49 | 2.42 | 18 | 8 |
| 1:A:45:THR:O | 1:A:129:MET:HE2 | 0.49 | 2.07 | 12 | 3 |
| 1:A:157:VAL:CG2 | 1:A:250:GLY:O | 0.49 | 2.60 | 18 | 2 |
| 1:A:139:GLY:C | 1:A:142:ARG:NH1 | 0.49 | 2.65 | 16 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:189:VAL:HG22 | 1:A:194:GLY:CA | 0.49 | 2.37 | 1 | 2 |
| 1:A:48:VAL:HG23 | 1:A:194:GLY:O | 0.49 | 2.07 | 2 | 3 |
| 1:A:66:LEU:CD2 | 1:A:66:LEU:C | 0.48 | 2.81 | 5 | 2 |
| 1:A:66:LEU:CD2 | 1:A:66:LEU:O | 0.48 | 2.62 | 1 | 1 |
| 1:A:101:LEU:O | 1:A:104:TYR:CE1 | 0.48 | 2.66 | 18 | 5 |
| 1:A:66:LEU:C | 1:A:66:LEU:CD2 | 0.48 | 2.81 | 11 | 2 |
| 1:A:4:VAL:HG21 | 1:A:178:LEU:HB3 | 0.48 | 1.85 | 13 | 1 |
| 1:A:128:ASP:OD2 | 1:A:142:ARG:NH1 | 0.48 | 2.46 | 5 | 1 |
| 1:A:25:THR:O | 1:A:42:HIS:ND1 | 0.48 | 2.47 | 19 | 6 |
| 1:A:187:GLN:HB2 | 1:A:195:HIS:O | 0.48 | 2.07 | 1 | 15 |
| 1:A:48:VAL:CG2 | 1:A:194:GLY:O | 0.48 | 2.62 | 17 | 5 |
| 1:A:129:MET:HE2 | 1:A:137:SER:HB2 | 0.48 | 1.86 | 10 | 6 |
| 1:A:127:VAL:O | 1:A:128:ASP:C | 0.48 | 2.51 | 4 | 20 |
| 1:A:154:ASN:HB2 | 1:A:252:LYS:O | 0.48 | 2.09 | 10 | 15 |
| 1:A:185:TYR:CD1 | 1:A:185:TYR:O | 0.48 | 2.65 | 18 | 6 |
| 1:A:96:ASN:OD1 | 1:A:98:ASN:N | 0.48 | 2.46 | 12 | 1 |
| 1:A:160:ILE:CG1 | 1:A:170:TRP:CZ3 | 0.48 | 2.97 | 6 | 1 |
| 1:A:46:GLY:HA2 | 1:A:135:SER:O | 0.48 | 2.07 | 8 | 17 |
| 1:A:142:ARG:H | 1:A:142:ARG:NH1 | 0.48 | 2.06 | 16 | 1 |
| 1:A:197:PHE:CD1 | 1:A:210:VAL:CG1 | 0.48 | 2.95 | 12 | 3 |
| 1:A:80:PHE:O | 1:A:81:ASN:C | 0.48 | 2.51 | 5 | 19 |
| 1:A:80:PHE:O | 1:A:81:ASN:O | 0.48 | 2.31 | 20 | 20 |
| 1:A:171:GLU:OE1 | 1:A:206:ASN:ND2 | 0.48 | 2.47 | 6 | 2 |
| 1:A:67:LYS:O | 1:A:150:ASN:CG | 0.48 | 2.52 | 1 | 1 |
| 1:A:166:SER:O | 1:A:170:TRP:N | 0.48 | 2.45 | 8 | 6 |
| 1:A:141:SER:O | 1:A:145:ARG:CB | 0.48 | 2.62 | 13 | 2 |
| 1:A:145:ARG:NH2 | 1:A:149:GLU:OE2 | 0.48 | 2.47 | 5 | 1 |
| 1:A:128:ASP:OD1 | 1:A:142:ARG:CD | 0.48 | 2.61 | 2 | 1 |
| 1:A:202:ALA:HA | 1:A:208:TYR:HA | 0.48 | 1.85 | 2 | 1 |
| 1:A:66:LEU:CB | 1:A:150:ASN:O | 0.48 | 2.61 | 5 | 3 |
| 1:A:108:GLU:N | 1:A:108:GLU:OE1 | 0.48 | 2.47 | 3 | 1 |
| 1:A:187:GLN:NE2 | 1:A:189:VAL:HG22 | 0.48 | 2.23 | 17 | 1 |
| 1:A:15:TYR:CD2 | 1:A:120:MET:HE1 | 0.48 | 2.44 | 16 | 1 |
| 1:A:16:ASN:HB3 | 1:A:21:TYR:CD2 | 0.48 | 2.43 | 16 | 2 |
| 1:A:46:GLY:CA | 1:A:135:SER:HB2 | 0.48 | 2.39 | 1 | 4 |
| 1:A:6:SER:OG | 1:A:9:ASP:CB | 0.48 | 2.62 | 5 | 4 |
| 1:A:6:SER:CA | 1:A:200:ASP:OD2 | 0.48 | 2.61 | 3 | 1 |
| 1:A:187:GLN:CG | 1:A:246:SER:O | 0.48 | 2.61 | 4 | 1 |
| 1:A:127:VAL:CB | 1:A:142:ARG:HB3 | 0.48 | 2.39 | 10 | 10 |
| 1:A:211:ASN:O | 1:A:212:TRP:O | 0.48 | 2.32 | 5 | 8 |
| 1:A:15:TYR:HA | 1:A:21:TYR:CZ | 0.47 | 2.44 | 7 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:43:ALA:CB | 1:A:131:TYR:HB3 | 0.47 | 2.39 | 15 | 14 |
| 1:A:79:TYR:CE1 | 1:A:133:PRO:CD | 0.47 | 2.97 | 3 | 5 |
| 1:A:20:PRO:HA | 1:A:23:LEU:CD1 | 0.47 | 2.39 | 5 | 3 |
| 1:A:210:VAL:CG1 | 1:A:211:ASN:N | 0.47 | 2.77 | 4 | 1 |
| 1:A:203:ASP:HB2 | 1:A:207:PHE:CB | 0.47 | 2.39 | 9 | 2 |
| 1:A:197:PHE:CD1 | 1:A:197:PHE:C | 0.47 | 2.87 | 20 | 4 |
| 1:A:183:PRO:HA | 1:A:199:ILE:O | 0.47 | 2.09 | 8 | 8 |
| 1:A:13:ILE:CD1 | 1:A:58:TYR:HA | 0.47 | 2.40 | 20 | 3 |
| 1:A:174:ILE:HA | 1:A:184:VAL:HG21 | 0.47 | 1.86 | 18 | 1 |
| 1:A:64:LYS:NZ | 1:A:64:LYS:CB | 0.47 | 2.77 | 17 | 1 |
| 1:A:160:ILE:O | 1:A:246:SER:HA | 0.47 | 2.10 | 4 | 17 |
| 1:A:148:LYS:O | 1:A:152:GLY:HA2 | 0.47 | 2.08 | 15 | 20 |
| 1:A:59:HIS:O | 1:A:60:ASN:OD1 | 0.47 | 2.32 | 9 | 9 |
| 1:A:163:GLY:N | 1:A:245:GLN:HG3 | 0.47 | 2.24 | 10 | 4 |
| 1:A:104:TYR:CE2 | 1:A:116:ILE:HB | 0.47 | 2.44 | 16 | 1 |
| 1:A:69:TYR:CE2 | 1:A:71:TYR:HD2 | 0.47 | 2.26 | 1 | 1 |
| 1:A:178:LEU:HD12 | 1:A:208:TYR:CD1 | 0.47 | 2.44 | 1 | 1 |
| 1:A:44:ALA:C | 1:A:135:SER:OG | 0.47 | 2.53 | 4 | 4 |
| 1:A:175:ASP:OD2 | 1:A:208:TYR:OH | 0.47 | 2.31 | 12 | 4 |
| 1:A:211:ASN:OD1 | 1:A:211:ASN:O | 0.47 | 2.32 | 20 | 2 |
| 1:A:94:GLN:CA | 1:A:94:GLN:NE2 | 0.47 | 2.77 | 13 | 3 |
| 1:A:175:ASP:OD1 | 1:A:208:TYR:CE2 | 0.47 | 2.67 | 3 | 3 |
| 1:A:175:ASP:OD1 | 1:A:208:TYR:OH | 0.47 | 2.32 | 3 | 3 |
| 1:A:197:PHE:C | 1:A:197:PHE:CD1 | 0.47 | 2.88 | 13 | 3 |
| 1:A:48:VAL:HG12 | 1:A:127:VAL:HG21 | 0.47 | 1.86 | 16 | 2 |
| 1:A:166:SER:OG | 1:A:169:ASP:OD2 | 0.47 | 2.33 | 16 | 1 |
| 1:A:127:VAL:CA | 1:A:142:ARG:HB3 | 0.47 | 2.39 | 7 | 10 |
| 1:A:69:TYR:CZ | 1:A:70:THR:HA | 0.47 | 2.44 | 1 | 1 |
| 1:A:140:SER:CB | 1:A:159:GLN:HG3 | 0.47 | 2.40 | 1 | 4 |
| 1:A:189:VAL:HG12 | 1:A:190:GLY:H | 0.47 | 1.69 | 18 | 4 |
| 1:A:16:ASN:HB3 | 1:A:21:TYR:CD1 | 0.47 | 2.45 | 3 | 1 |
| 1:A:49:ALA:HB2 | 1:A:124:GLY:HA2 | 0.47 | 1.87 | 16 | 4 |
| 1:A:61:TYR:HB3 | 1:A:153:TYR:CZ | 0.47 | 2.45 | 18 | 2 |
| 1:A:61:TYR:CG | 1:A:253:PRO:HB3 | 0.47 | 2.45 | 9 | 2 |
| 1:A:61:TYR:CE1 | 1:A:253:PRO:HB3 | 0.47 | 2.45 | 18 | 1 |
| 1:A:139:GLY:O | 1:A:142:ARG:CZ | 0.47 | 2.62 | 16 | 1 |
| 1:A:160:ILE:O | 1:A:246:SER:HB2 | 0.47 | 2.10 | 20 | 9 |
| 1:A:76:ASN:O | 1:A:78:PRO:HD3 | 0.47 | 2.10 | 2 | 19 |
| 1:A:90:ILE:O | 1:A:91:SER:C | 0.47 | 2.53 | 3 | 20 |
| 1:A:95:TYR:HH | 1:A:151:PHE:HE1 | 0.47 | 1.51 | 13 | 4 |
| 1:A:118:GLU:O | 1:A:122:ASP:OD1 | 0.47 | 2.33 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:101:LEU:O | 1:A:104:TYR:CE2 | 0.47 | 2.67 | 9 | 1 |
| 1:A:16:ASN:CB | 1:A:21:TYR:CE1 | 0.47 | 2.97 | 6 | 1 |
| 1:A:28:ILE:HD11 | 1:A:132:GLY:CA | 0.47 | 2.40 | 18 | 16 |
| 1:A:211:ASN:O | 1:A:211:ASN:OD1 | 0.47 | 2.33 | 10 | 5 |
| 1:A:66:LEU:CD1 | 1:A:152:GLY:HA3 | 0.47 | 2.40 | 15 | 1 |
| 1:A:17:GLN:NE2 | 1:A:47:SER:HA | 0.47 | 2.25 | 18 | 2 |
| 1:A:125:ILE:O | 1:A:128:ASP:N | 0.47 | 2.47 | 5 | 8 |
| 1:A:185:TYR:HD2 | 1:A:248:VAL:HG23 | 0.47 | 1.69 | 14 | 1 |
| 1:A:140:SER:CB | 1:A:159:GLN:CD | 0.47 | 2.83 | 15 | 2 |
| 1:A:116:ILE:O | 1:A:120:MET:CG | 0.47 | 2.63 | 2 | 1 |
| 1:A:162:ARG:CD | 1:A:170:TRP:CD1 | 0.46 | 2.98 | 14 | 2 |
| 1:A:187:GLN:NE2 | 1:A:189:VAL:HG23 | 0.46 | 2.24 | 15 | 1 |
| 1:A:212:TRP:CE3 | 1:A:212:TRP:HA | 0.46 | 2.44 | 19 | 1 |
| 1:A:53:ALA:HB1 | 1:A:119:LEU:CD2 | 0.46 | 2.40 | 19 | 8 |
| 1:A:88:ALA:O | 1:A:90:ILE:N | 0.46 | 2.47 | 17 | 8 |
| 1:A:6:SER:HA | 1:A:200:ASP:O | 0.46 | 2.09 | 1 | 3 |
| 1:A:100:ILE:HG22 | 1:A:100:ILE:O | 0.46 | 2.10 | 17 | 1 |
| 1:A:52:THR:HB | 1:A:123:VAL:HG11 | 0.46 | 1.87 | 16 | 1 |
| 1:A:171:GLU:O | 1:A:175:ASP:OD1 | 0.46 | 2.32 | 3 | 3 |
| 1:A:13:ILE:HG12 | 1:A:57:LYS:CG | 0.46 | 2.40 | 15 | 1 |
| 1:A:188:GLY:O | 1:A:195:HIS:N | 0.46 | 2.44 | 3 | 1 |
| 1:A:95:TYR:OH | 1:A:122:ASP:CB | 0.46 | 2.63 | 9 | 3 |
| 1:A:4:VAL:N | 1:A:202:ALA:O | 0.46 | 2.43 | 3 | 1 |
| 1:A:87:PHE:CZ | 1:A:89:ALA:HA | 0.46 | 2.45 | 20 | 1 |
| 1:A:81:ASN:N | 1:A:81:ASN:ND2 | 0.46 | 2.63 | 18 | 1 |
| 1:A:11:LYS:CD | 1:A:58:TYR:CD2 | 0.46 | 2.98 | 10 | 1 |
| 1:A:177:GLU:OE1 | 1:A:250:GLY:N | 0.46 | 2.48 | 6 | 3 |
| 1:A:205:ARG:O | 1:A:206:ASN:C | 0.46 | 2.54 | 1 | 1 |
| 1:A:53:ALA:HA | 1:A:56:MET:HB2 | 0.46 | 1.88 | 10 | 4 |
| 1:A:140:SER:O | 1:A:144:GLN:CG | 0.46 | 2.64 | 14 | 5 |
| 1:A:57:LYS:O | 1:A:60:ASN:OD1 | 0.46 | 2.33 | 19 | 2 |
| 1:A:19:ASN:ND2 | 1:A:106:GLY:HA3 | 0.46 | 2.26 | 16 | 1 |
| 1:A:15:TYR:HB2 | 1:A:54:GLN:HG2 | 0.46 | 1.87 | 1 | 13 |
| 1:A:26:PRO:CG | 1:A:131:TYR:CG | 0.46 | 2.98 | 6 | 11 |
| 1:A:47:SER:O | 1:A:51:ALA:N | 0.46 | 2.41 | 16 | 8 |
| 1:A:6:SER:HB2 | 1:A:209:HIS:ND1 | 0.46 | 2.25 | 18 | 4 |
| 1:A:67:LYS:O | 1:A:90:ILE:HB | 0.46 | 2.11 | 18 | 12 |
| 1:A:4:VAL:CG2 | 1:A:202:ALA:HB3 | 0.46 | 2.37 | 3 | 1 |
| 1:A:52:THR:CG2 | 1:A:147:LEU:HD21 | 0.46 | 2.40 | 2 | 1 |
| 1:A:78:PRO:HD2 | 1:A:79:TYR:CE2 | 0.46 | 2.46 | 19 | 7 |
| 1:A:118:GLU:O | 1:A:122:ASP:CG | 0.46 | 2.54 | 16 | 19 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:151:PHE:O | 1:A:152:GLY:C | 0.46 | 2.54 | 17 | 9 |
| 1:A:173:GLN:NE2 | 1:A:249:VAL:HG21 | 0.46 | 2.26 | 10 | 4 |
| 1:A:69:TYR:HB3 | 1:A:150:ASN:ND2 | 0.46 | 2.26 | 1 | 1 |
| 1:A:162:ARG:HB3 | 1:A:245:GLN:CB | 0.46 | 2.41 | 14 | 4 |
| 1:A:92:THR:OG1 | 1:A:92:THR:O | 0.46 | 2.30 | 3 | 2 |
| 1:A:140:SER:N | 1:A:187:GLN:OE1 | 0.46 | 2.40 | 13 | 2 |
| 1:A:55:ILE:HG21 | 1:A:251:ILE:CD1 | 0.46 | 2.41 | 13 | 2 |
| 1:A:124:GLY:O | 1:A:129:MET:HB2 | 0.46 | 2.10 | 18 | 14 |
| 1:A:25:THR:HB | 1:A:26:PRO:HD2 | 0.46 | 1.87 | 6 | 14 |
| 1:A:180:GLN:O | 1:A:182:GLN:HG3 | 0.46 | 2.10 | 10 | 9 |
| 1:A:60:ASN:CG | 1:A:97:TRP:CE3 | 0.46 | 2.89 | 19 | 1 |
| 1:A:159:GLN:HG2 | 1:A:160:ILE:N | 0.46 | 2.26 | 20 | 4 |
| 1:A:51:ALA:O | 1:A:198:VAL:CG2 | 0.46 | 2.64 | 18 | 5 |
| 1:A:128:ASP:OD1 | 1:A:142:ARG:HD2 | 0.46 | 2.11 | 2 | 1 |
| 1:A:22:ASN:OD1 | 1:A:22:ASN:C | 0.46 | 2.54 | 6 | 8 |
| 1:A:69:TYR:CG | 1:A:126:SER:HA | 0.46 | 2.45 | 6 | 5 |
| 1:A:46:GLY:HA3 | 1:A:129:MET:HE3 | 0.46 | 1.86 | 3 | 5 |
| 1:A:129:MET:SD | 1:A:137:SER:HB2 | 0.46 | 2.51 | 14 | 5 |
| 1:A:7:LEU:HD13 | 1:A:183:PRO:HD3 | 0.46 | 1.88 | 3 | 2 |
| 1:A:130:ASP:N | 1:A:136:GLY:O | 0.46 | 2.44 | 20 | 1 |
| 1:A:20:PRO:CB | 1:A:113:LYS:HG2 | 0.46 | 2.41 | 7 | 12 |
| 1:A:121:ALA:O | 1:A:125:ILE:HB | 0.46 | 2.11 | 14 | 16 |
| 1:A:46:GLY:HA3 | 1:A:129:MET:SD | 0.46 | 2.50 | 16 | 13 |
| 1:A:6:SER:OG | 1:A:9:ASP:HB2 | 0.46 | 2.11 | 5 | 4 |
| 1:A:171:GLU:O | 1:A:174:ILE:N | 0.46 | 2.48 | 17 | 2 |
| 1:A:171:GLU:OE2 | 1:A:206:ASN:OD1 | 0.46 | 2.34 | 10 | 1 |
| 1:A:140:SER:O | 1:A:144:GLN:HG3 | 0.45 | 2.12 | 9 | 7 |
| 1:A:17:GLN:HG2 | 1:A:50:THR:OG1 | 0.45 | 2.11 | 16 | 11 |
| 1:A:147:LEU:HD12 | 1:A:248:VAL:HG11 | 0.45 | 1.87 | 7 | 2 |
| 1:A:178:LEU:O | 1:A:181:ASN:N | 0.45 | 2.47 | 5 | 2 |
| 1:A:45:THR:CB | 1:A:120:MET:SD | 0.45 | 3.05 | 6 | 5 |
| 1:A:18:GLY:O | 1:A:22:ASN:CG | 0.45 | 2.54 | 12 | 13 |
| 1:A:64:LYS:HG2 | 1:A:93:ARG:O | 0.45 | 2.11 | 1 | 2 |
| 1:A:177:GLU:OE1 | 1:A:182:GLN:HB3 | 0.45 | 2.10 | 18 | 3 |
| 1:A:145:ARG:CG | 1:A:149:GLU:CD | 0.45 | 2.85 | 16 | 3 |
| 1:A:13:ILE:HA | 1:A:102:PRO:HB2 | 0.45 | 1.89 | 18 | 3 |
| 1:A:107:ARG:HD3 | 1:A:107:ARG:O | 0.45 | 2.10 | 19 | 1 |
| 1:A:180:GLN:O | 1:A:182:GLN:HG2 | 0.45 | 2.11 | 13 | 1 |
| 1:A:199:ILE:HG21 | 1:A:208:TYR:HD2 | 0.45 | 1.69 | 13 | 1 |
| 1:A:107:ARG:C | 1:A:107:ARG:HE | 0.45 | 2.14 | 17 | 1 |
| 1:A:26:PRO:HG2 | 1:A:131:TYR:CB | 0.45 | 2.42 | 8 | 14 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:58:TYR:O | 1:A:58:TYR:CD1 | 0.45 | 2.69 | 6 | 1 |
| 1:A:60:ASN:HA | 1:A:97:TRP:CZ2 | 0.45 | 2.47 | 12 | 3 |
| 1:A:28:ILE:HG22 | 1:A:39:VAL:HA | 0.45 | 1.86 | 17 | 5 |
| 1:A:69:TYR:OH | 1:A:128:ASP:OD1 | 0.45 | 2.32 | 7 | 3 |
| 1:A:15:TYR:CE2 | 1:A:54:GLN:HA | 0.45 | 2.47 | 19 | 2 |
| 1:A:141:SER:O | 1:A:145:ARG:HB2 | 0.45 | 2.11 | 13 | 2 |
| 1:A:57:LYS:HD3 | 1:A:100:ILE:O | 0.45 | 2.11 | 13 | 3 |
| 1:A:43:ALA:HA | 1:A:132:GLY:O | 0.45 | 2.11 | 20 | 10 |
| 1:A:160:ILE:HG21 | 1:A:173:GLN:HE21 | 0.45 | 1.71 | 8 | 1 |
| 1:A:7:LEU:O | 1:A:10:SER:OG | 0.45 | 2.32 | 8 | 1 |
| 1:A:16:ASN:OD1 | 1:A:17:GLN:N | 0.45 | 2.46 | 3 | 1 |
| 1:A:180:GLN:O | 1:A:181:ASN:C | 0.45 | 2.55 | 5 | 8 |
| 1:A:118:GLU:O | 1:A:122:ASP:OD2 | 0.45 | 2.33 | 19 | 2 |
| 1:A:178:LEU:HD12 | 1:A:208:TYR:CE2 | 0.45 | 2.46 | 13 | 1 |
| 1:A:189:VAL:HG22 | 1:A:194:GLY:HA2 | 0.45 | 1.89 | 9 | 4 |
| 1:A:22:ASN:C | 1:A:22:ASN:OD1 | 0.45 | 2.53 | 10 | 12 |
| 1:A:171:GLU:HA | 1:A:174:ILE:HD12 | 0.45 | 1.88 | 15 | 6 |
| 1:A:147:LEU:HB2 | 1:A:157:VAL:HG11 | 0.45 | 1.88 | 13 | 8 |
| 1:A:53:ALA:HB1 | 1:A:119:LEU:HD21 | 0.45 | 1.87 | 20 | 5 |
| 1:A:144:GLN:HG3 | 1:A:145:ARG:N | 0.45 | 2.27 | 19 | 2 |
| 1:A:71:TYR:HB3 | 1:A:128:ASP:OD1 | 0.45 | 2.12 | 13 | 2 |
| 1:A:11:LYS:O | 1:A:102:PRO:CB | 0.45 | 2.64 | 18 | 1 |
| 1:A:38:PHE:CE2 | 1:A:133:PRO:HG3 | 0.45 | 2.46 | 16 | 1 |
| 1:A:140:SER:CB | 1:A:159:GLN:OE1 | 0.45 | 2.65 | 6 | 1 |
| 1:A:7:LEU:HG | 1:A:200:ASP:O | 0.45 | 2.12 | 1 | 6 |
| 1:A:19:ASN:HB3 | 1:A:21:TYR:CE2 | 0.45 | 2.47 | 1 | 1 |
| 1:A:50:THR:O | 1:A:54:GLN:HG3 | 0.45 | 2.12 | 14 | 12 |
| 1:A:93:ARG:NE | 1:A:118:GLU:OE2 | 0.45 | 2.50 | 8 | 1 |
| 1:A:13:ILE:HA | 1:A:102:PRO:O | 0.45 | 2.12 | 18 | 5 |
| 1:A:162:ARG:HG2 | 1:A:245:GLN:NE2 | 0.45 | 2.25 | 13 | 3 |
| 1:A:110:ASN:N | 1:A:110:ASN:OD1 | 0.45 | 2.49 | 7 | 1 |
| 1:A:69:TYR:CE1 | 1:A:87:PHE:HA | 0.45 | 2.46 | 1 | 1 |
| 1:A:82:HIS:H | 1:A:83:PRO:HD2 | 0.45 | 1.72 | 3 | 6 |
| 1:A:27:VAL:O | 1:A:80:PHE:CZ | 0.45 | 2.69 | 12 | 1 |
| 1:A:119:LEU:O | 1:A:123:VAL:HG23 | 0.45 | 2.12 | 3 | 6 |
| 1:A:107:ARG:NE | 1:A:107:ARG:C | 0.45 | 2.70 | 17 | 1 |
| 1:A:31:VAL:CG2 | 1:A:37:SER:OG | 0.45 | 2.65 | 4 | 1 |
| 1:A:186:TYR:CB | 1:A:197:PHE:CE1 | 0.45 | 3.00 | 6 | 3 |
| 1:A:66:LEU:O | 1:A:66:LEU:HD22 | 0.45 | 2.12 | 1 | 1 |
| 1:A:187:GLN:O | 1:A:187:GLN:HG3 | 0.45 | 2.12 | 8 | 4 |
| 1:A:187:GLN:CB | 1:A:196:ALA:HA | 0.45 | 2.41 | 3 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:200:ASP:OD1 | 1:A:200:ASP:C | 0.45 | 2.55 | 13 | 1 |
| 1:A:80:PHE:CE1 | 1:A:131:TYR:O | 0.45 | 2.70 | 13 | 1 |
| 1:A:14:HIS:CD2 | 1:A:103:THR:HB | 0.45 | 2.47 | 17 | 1 |
| 1:A:176:LYS:HB3 | 1:A:176:LYS:NZ | 0.45 | 2.17 | 5 | 1 |
| 1:A:171:GLU:HG2 | 1:A:208:TYR:CZ | 0.45 | 2.47 | 11 | 1 |
| 1:A:11:LYS:O | 1:A:12:GLY:C | 0.45 | 2.55 | 6 | 18 |
| 1:A:57:LYS:HE2 | 1:A:102:PRO:N | 0.45 | 2.27 | 20 | 18 |
| 1:A:93:ARG:NE | 1:A:118:GLU:CD | 0.45 | 2.71 | 1 | 1 |
| 1:A:45:THR:CG2 | 1:A:120:MET:SD | 0.45 | 2.95 | 7 | 7 |
| 1:A:27:VAL:O | 1:A:80:PHE:CE2 | 0.45 | 2.70 | 17 | 2 |
| 1:A:66:LEU:HB3 | 1:A:150:ASN:O | 0.45 | 2.12 | 5 | 2 |
| 1:A:81:ASN:O | 1:A:82:HIS:CB | 0.45 | 2.64 | 5 | 20 |
| 1:A:71:TYR:OH | 1:A:131:TYR:CD2 | 0.45 | 2.70 | 6 | 1 |
| 1:A:140:SER:HB2 | 1:A:159:GLN:OE1 | 0.45 | 2.12 | 6 | 4 |
| 1:A:94:GLN:NE2 | 1:A:94:GLN:HA | 0.45 | 2.25 | 6 | 1 |
| 1:A:154:ASN:ND2 | 1:A:156:SER:HB3 | 0.45 | 2.27 | 12 | 1 |
| 1:A:118:GLU:O | 1:A:122:ASP:N | 0.45 | 2.41 | 12 | 2 |
| 1:A:144:GLN:HA | 1:A:157:VAL:CG1 | 0.45 | 2.42 | 13 | 1 |
| 1:A:178:LEU:HD22 | 1:A:201:GLY:N | 0.45 | 2.27 | 10 | 1 |
| 1:A:130:ASP:HB2 | 1:A:136:GLY:O | 0.44 | 2.11 | 5 | 4 |
| 1:A:129:MET:SD | 1:A:137:SER:CB | 0.44 | 3.05 | 14 | 2 |
| 1:A:101:LEU:HD12 | 1:A:108:GLU:HG2 | 0.44 | 1.88 | 18 | 1 |
| 1:A:185:TYR:O | 1:A:247:ALA:HB1 | 0.44 | 2.12 | 7 | 2 |
| 1:A:201:GLY:O | 1:A:208:TYR:CG | 0.44 | 2.70 | 13 | 1 |
| 1:A:175:ASP:CG | 1:A:208:TYR:OH | 0.44 | 2.56 | 13 | 1 |
| 1:A:177:GLU:O | 1:A:182:GLN:HB2 | 0.44 | 2.12 | 19 | 14 |
| 1:A:19:ASN:HB3 | 1:A:21:TYR:CD1 | 0.44 | 2.48 | 5 | 7 |
| 1:A:6:SER:CB | 1:A:9:ASP:HB2 | 0.44 | 2.43 | 6 | 8 |
| 1:A:20:PRO:HB3 | 1:A:113:LYS:CD | 0.44 | 2.41 | 8 | 1 |
| 1:A:17:GLN:O | 1:A:45:THR:HG23 | 0.44 | 2.12 | 9 | 4 |
| 1:A:17:GLN:O | 1:A:22:ASN:HB3 | 0.44 | 2.12 | 3 | 9 |
| 1:A:61:TYR:CE2 | 1:A:151:PHE:O | 0.44 | 2.70 | 4 | 12 |
| 1:A:211:ASN:C | 1:A:211:ASN:OD1 | 0.44 | 2.56 | 6 | 2 |
| 1:A:189:VAL:HG13 | 1:A:194:GLY:N | 0.44 | 2.27 | 3 | 1 |
| 1:A:185:TYR:CD1 | 1:A:248:VAL:CB | 0.44 | 3.00 | 18 | 1 |
| 1:A:203:ASP:O | 1:A:205:ARG:N | 0.44 | 2.51 | 5 | 2 |
| 1:A:7:LEU:HB3 | 1:A:58:TYR:CZ | 0.44 | 2.47 | 13 | 3 |
| 1:A:30:LYS:CB | 1:A:78:PRO:O | 0.44 | 2.66 | 18 | 2 |
| 1:A:68:ASP:OD1 | 1:A:91:SER:CB | 0.44 | 2.65 | 9 | 2 |
| 1:A:211:ASN:OD1 | 1:A:211:ASN:C | 0.44 | 2.56 | 20 | 3 |
| 1:A:15:TYR:OH | 1:A:57:LYS:HD3 | 0.44 | 2.11 | 7 | 9 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:93:ARG:CD | 1:A:118:GLU:OE2 | 0.44 | 2.65 | 13 | 2 |
| 1:A:113:LYS:O | 1:A:117:SER:CB | 0.44 | 2.65 | 12 | 1 |
| 1:A:60:ASN:HA | 1:A:97:TRP:CH2 | 0.44 | 2.47 | 12 | 1 |
| 1:A:29:GLU:C | 1:A:39:VAL:HG22 | 0.44 | 2.32 | 15 | 2 |
| 1:A:44:ALA:N | 1:A:132:GLY:O | 0.44 | 2.44 | 4 | 1 |
| 1:A:18:GLY:HA2 | 1:A:22:ASN:ND2 | 0.44 | 2.28 | 20 | 2 |
| 1:A:25:THR:OG1 | 1:A:43:ALA:O | 0.44 | 2.30 | 4 | 2 |
| 1:A:93:ARG:NE | 1:A:118:GLU:HG3 | 0.44 | 2.28 | 11 | 1 |
| 1:A:90:ILE:HA | 1:A:93:ARG:HG3 | 0.44 | 1.90 | 1 | 13 |
| 1:A:116:ILE:O | 1:A:120:MET:HG2 | 0.44 | 2.13 | 10 | 4 |
| 1:A:109:SER:OG | 1:A:110:ASN:N | 0.44 | 2.49 | 2 | 2 |
| 1:A:19:ASN:ND2 | 1:A:21:TYR:CD2 | 0.44 | 2.86 | 18 | 1 |
| 1:A:202:ALA:HB2 | 1:A:208:TYR:CZ | 0.44 | 2.47 | 13 | 1 |
| 1:A:109:SER:CB | 1:A:112:GLN:OE1 | 0.44 | 2.66 | 3 | 2 |
| 1:A:160:ILE:HG12 | 1:A:247:ALA:O | 0.44 | 2.13 | 6 | 3 |
| 1:A:68:ASP:N | 1:A:91:SER:HB3 | 0.44 | 2.28 | 1 | 1 |
| 1:A:46:GLY:N | 1:A:135:SER:HB2 | 0.44 | 2.28 | 1 | 1 |
| 1:A:6:SER:OG | 1:A:9:ASP:CG | 0.44 | 2.56 | 20 | 3 |
| 1:A:6:SER:HA | 1:A:200:ASP:OD1 | 0.44 | 2.13 | 19 | 5 |
| 1:A:129:MET:HB3 | 1:A:131:TYR:CE2 | 0.44 | 2.48 | 3 | 1 |
| 1:A:161:ASN:CB | 1:A:164:ASP:OD2 | 0.44 | 2.66 | 13 | 1 |
| 1:A:110:ASN:OD1 | 1:A:110:ASN:N | 0.43 | 2.51 | 1 | 1 |
| 1:A:161:ASN:O | 1:A:164:ASP:N | 0.43 | 2.44 | 5 | 2 |
| 1:A:129:MET:HE1 | 1:A:137:SER:HB2 | 0.43 | 1.90 | 3 | 2 |
| 1:A:139:GLY:HA3 | 1:A:187:GLN:NE2 | 0.43 | 2.28 | 5 | 3 |
| 1:A:13:ILE:CD1 | 1:A:58:TYR:CA | 0.43 | 2.96 | 20 | 1 |
| 1:A:94:GLN:HA | 1:A:94:GLN:NE2 | 0.43 | 2.28 | 20 | 1 |
| 1:A:61:TYR:CG | 1:A:62:PRO:HD3 | 0.43 | 2.48 | 16 | 4 |
| 1:A:64:LYS:HB2 | 1:A:64:LYS:NZ | 0.43 | 2.28 | 17 | 1 |
| 1:A:127:VAL:C | 1:A:128:ASP:OD1 | 0.43 | 2.56 | 2 | 1 |
| 1:A:126:SER:OG | 1:A:146:ALA:CB | 0.43 | 2.65 | 1 | 3 |
| 1:A:177:GLU:HB3 | 1:A:182:GLN:O | 0.43 | 2.14 | 17 | 8 |
| 1:A:130:ASP:O | 1:A:135:SER:HA | 0.43 | 2.13 | 2 | 5 |
| 1:A:161:ASN:HB3 | 1:A:164:ASP:OD2 | 0.43 | 2.13 | 13 | 2 |
| 1:A:31:VAL:HG23 | 1:A:39:VAL:HG23 | 0.43 | 1.89 | 7 | 3 |
| 1:A:93:ARG:NH2 | 1:A:118:GLU:OE2 | 0.43 | 2.52 | 17 | 1 |
| 1:A:26:PRO:CG | 1:A:131:TYR:CD2 | 0.43 | 3.01 | 12 | 4 |
| 1:A:187:GLN:NE2 | 1:A:189:VAL:CG2 | 0.43 | 2.81 | 16 | 3 |
| 1:A:21:TYR:HB3 | 1:A:120:MET:HG3 | 0.43 | 1.90 | 3 | 5 |
| 1:A:30:LYS:HD3 | 1:A:80:PHE:O | 0.43 | 2.13 | 12 | 1 |
| 1:A:7:LEU:CB | 1:A:200:ASP:HB2 | 0.43 | 2.43 | 16 | 7 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:86:LEU:CD1 | 1:A:86:LEU:N | 0.43 | 2.79 | 15 | 2 |
| 1:A:140:SER:HB2 | 1:A:159:GLN:CD | 0.43 | 2.34 | 15 | 3 |
| 1:A:8:LEU:HD11 | 1:A:198:VAL:CG1 | 0.43 | 2.43 | 3 | 4 |
| 1:A:52:THR:O | 1:A:56:MET:HG3 | 0.43 | 2.13 | 4 | 2 |
| 1:A:188:GLY:N | 1:A:195:HIS:O | 0.43 | 2.43 | 4 | 1 |
| 1:A:130:ASP:CG | 1:A:136:GLY:O | 0.43 | 2.57 | 1 | 1 |
| 1:A:23:LEU:CD1 | 1:A:113:LYS:HD3 | 0.43 | 2.43 | 12 | 1 |
| 1:A:162:ARG:HB2 | 1:A:186:TYR:OH | 0.43 | 2.13 | 16 | 2 |
| 1:A:68:ASP:OD1 | 1:A:89:ALA:C | 0.43 | 2.57 | 4 | 4 |
| 1:A:6:SER:CB | 1:A:9:ASP:CB | 0.43 | 2.97 | 3 | 1 |
| 1:A:11:LYS:CD | 1:A:58:TYR:CE1 | 0.43 | 3.01 | 17 | 1 |
| 1:A:107:ARG:O | 1:A:107:ARG:HD3 | 0.43 | 2.14 | 10 | 1 |
| 1:A:94:GLN:NE2 | 1:A:94:GLN:CA | 0.43 | 2.81 | 2 | 1 |
| 1:A:47:SER:O | 1:A:48:VAL:C | 0.43 | 2.56 | 16 | 10 |
| 1:A:140:SER:O | 1:A:141:SER:C | 0.43 | 2.56 | 1 | 12 |
| 1:A:52:THR:HG22 | 1:A:56:MET:HG3 | 0.43 | 1.90 | 3 | 3 |
| 1:A:116:ILE:O | 1:A:117:SER:C | 0.43 | 2.56 | 18 | 2 |
| 1:A:164:ASP:N | 1:A:164:ASP:OD1 | 0.43 | 2.52 | 5 | 3 |
| 1:A:92:THR:O | 1:A:92:THR:OG1 | 0.43 | 2.37 | 17 | 2 |
| 1:A:195:HIS:ND1 | 1:A:212:TRP:CZ3 | 0.43 | 2.86 | 19 | 1 |
| 1:A:11:LYS:HD3 | 1:A:58:TYR:CD1 | 0.43 | 2.48 | 17 | 1 |
| 1:A:122:ASP:O | 1:A:126:SER:HB3 | 0.43 | 2.13 | 7 | 9 |
| 1:A:158:HIS:ND1 | 1:A:158:HIS:N | 0.43 | 2.66 | 1 | 4 |
| 1:A:90:ILE:O | 1:A:92:THR:N | 0.43 | 2.52 | 1 | 14 |
| 1:A:205:ARG:O | 1:A:206:ASN:HB2 | 0.43 | 2.12 | 20 | 3 |
| 1:A:107:ARG:O | 1:A:107:ARG:HD2 | 0.43 | 2.13 | 17 | 2 |
| 1:A:114:MET:HA | 1:A:117:SER:OG | 0.43 | 2.14 | 2 | 7 |
| 1:A:145:ARG:CD | 1:A:149:GLU:OE1 | 0.43 | 2.66 | 12 | 1 |
| 1:A:160:ILE:HD12 | 1:A:170:TRP:CZ2 | 0.43 | 2.46 | 14 | 1 |
| 1:A:171:GLU:HB3 | 1:A:208:TYR:OH | 0.43 | 2.13 | 16 | 7 |
| 1:A:22:ASN:HB2 | 1:A:43:ALA:O | 0.43 | 2.14 | 1 | 1 |
| 1:A:188:GLY:HA2 | 1:A:245:GLN:OE1 | 0.43 | 2.14 | 15 | 1 |
| 1:A:15:TYR:CZ | 1:A:57:LYS:HB2 | 0.43 | 2.49 | 15 | 1 |
| 1:A:21:TYR:CD1 | 1:A:116:ILE:CG1 | 0.43 | 3.01 | 20 | 1 |
| 1:A:106:GLY:O | 1:A:113:LYS:NZ | 0.43 | 2.43 | 16 | 2 |
| 1:A:11:LYS:HB2 | 1:A:13:ILE:HG13 | 0.43 | 1.90 | 18 | 3 |
| 1:A:174:ILE:HG23 | 1:A:199:ILE:HG21 | 0.43 | 1.90 | 18 | 1 |
| 1:A:38:PHE:HD2 | 1:A:79:TYR:CE1 | 0.43 | 2.29 | 13 | 3 |
| 1:A:162:ARG:HG3 | 1:A:245:GLN:OE1 | 0.43 | 2.13 | 4 | 1 |
| 1:A:202:ALA:HA | 1:A:207:PHE:O | 0.43 | 2.14 | 1 | 6 |
| 1:A:65:GLY:HA3 | 1:A:90:ILE:HG22 | 0.43 | 1.91 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:153:TYR:O | 1:A:154:ASN:C | 0.43 | 2.57 | 10 | 7 |
| 1:A:7:LEU:N | 1:A:200:ASP:HB2 | 0.43 | 2.29 | 16 | 4 |
| 1:A:70:THR:HA | 1:A:86:LEU:O | 0.43 | 2.14 | 4 | 4 |
| 1:A:64:LYS:HA | 1:A:93:ARG:O | 0.43 | 2.13 | 16 | 4 |
| 1:A:8:LEU:HD12 | 1:A:211:ASN:HB2 | 0.43 | 1.89 | 17 | 1 |
| 1:A:171:GLU:HG2 | 1:A:208:TYR:OH | 0.43 | 2.14 | 16 | 1 |
| 1:A:21:TYR:CE2 | 1:A:104:TYR:CD1 | 0.42 | 3.07 | 3 | 1 |
| 1:A:178:LEU:HD11 | 1:A:199:ILE:HG22 | 0.42 | 1.90 | 3 | 1 |
| 1:A:203:ASP:O | 1:A:204:GLY:C | 0.42 | 2.55 | 5 | 2 |
| 1:A:197:PHE:CE2 | 1:A:212:TRP:CZ3 | 0.42 | 3.07 | 2 | 1 |
| 1:A:98:ASN:OD1 | 1:A:98:ASN:O | 0.42 | 2.36 | 1 | 1 |
| 1:A:161:ASN:C | 1:A:170:TRP:CZ3 | 0.42 | 2.92 | 8 | 1 |
| 1:A:127:VAL:HB | 1:A:142:ARG:HB3 | 0.42 | 1.91 | 10 | 5 |
| 1:A:6:SER:HB2 | 1:A:9:ASP:HB3 | 0.42 | 1.91 | 3 | 3 |
| 1:A:178:LEU:HD21 | 1:A:199:ILE:O | 0.42 | 2.12 | 4 | 2 |
| 1:A:157:VAL:HG22 | 1:A:251:ILE:HA | 0.42 | 1.91 | 5 | 2 |
| 1:A:107:ARG:C | 1:A:107:ARG:CD | 0.42 | 2.87 | 8 | 1 |
| 1:A:187:GLN:HA | 1:A:196:ALA:HA | 0.42 | 1.90 | 3 | 1 |
| 1:A:8:LEU:HD11 | 1:A:198:VAL:CB | 0.42 | 2.44 | 17 | 1 |
| 1:A:210:VAL:CG1 | 1:A:212:TRP:CD2 | 0.42 | 3.03 | 4 | 1 |
| 1:A:93:ARG:HD3 | 1:A:118:GLU:OE2 | 0.42 | 2.14 | 12 | 1 |
| 1:A:69:TYR:HB2 | 1:A:150:ASN:ND2 | 0.42 | 2.29 | 4 | 4 |
| 1:A:49:ALA:HA | 1:A:123:VAL:HG12 | 0.42 | 1.90 | 16 | 1 |
| 1:A:116:ILE:O | 1:A:120:MET:HG3 | 0.42 | 2.14 | 2 | 1 |
| 1:A:113:LYS:O | 1:A:117:SER:HB3 | 0.42 | 2.15 | 13 | 4 |
| 1:A:88:ALA:CB | 1:A:90:ILE:HG13 | 0.42 | 2.45 | 1 | 1 |
| 1:A:89:ALA:CB | 1:A:92:THR:HG23 | 0.42 | 2.39 | 3 | 2 |
| 1:A:145:ARG:O | 1:A:149:GLU:HB2 | 0.42 | 2.14 | 7 | 1 |
| 1:A:174:ILE:HG12 | 1:A:184:VAL:HG11 | 0.42 | 1.92 | 17 | 1 |
| 1:A:197:PHE:HB2 | 1:A:211:ASN:O | 0.42 | 2.14 | 12 | 1 |
| 1:A:124:GLY:HA2 | 1:A:127:VAL:HG22 | 0.42 | 1.89 | 20 | 1 |
| 1:A:55:ILE:HD13 | 1:A:251:ILE:HD13 | 0.42 | 1.90 | 17 | 1 |
| 1:A:161:ASN:O | 1:A:163:GLY:N | 0.42 | 2.52 | 10 | 1 |
| 1:A:140:SER:HA | 1:A:248:VAL:CG2 | 0.42 | 2.45 | 1 | 1 |
| 1:A:147:LEU:CD1 | 1:A:251:ILE:HG12 | 0.42 | 2.42 | 7 | 1 |
| 1:A:162:ARG:HD3 | 1:A:170:TRP:CG | 0.42 | 2.50 | 4 | 1 |
| 1:A:38:PHE:HB3 | 1:A:41:GLN:NE2 | 0.42 | 2.30 | 4 | 2 |
| 1:A:142:ARG:HG3 | 1:A:142:ARG:HH11 | 0.42 | 1.73 | 16 | 1 |
| 1:A:58:TYR:CD1 | 1:A:58:TYR:C | 0.42 | 2.93 | 19 | 3 |
| 1:A:139:GLY:HA3 | 1:A:187:GLN:CD | 0.42 | 2.35 | 2 | 4 |
| 1:A:72:THR:O | 1:A:73:LEU:C | 0.42 | 2.58 | 13 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:148:LYS:NZ | 1:A:157:VAL:O | 0.42 | 2.49 | 19 | 1 |
| 1:A:21:TYR:CE1 | 1:A:104:TYR:CD1 | 0.42 | 3.08 | 18 | 1 |
| 1:A:177:GLU:OE1 | 1:A:177:GLU:HA | 0.42 | 2.14 | 13 | 1 |
| 1:A:50:THR:HG23 | 1:A:120:MET:HE3 | 0.42 | 1.90 | 2 | 2 |
| 1:A:69:TYR:CD1 | 1:A:126:SER:HA | 0.42 | 2.49 | 6 | 3 |
| 1:A:142:ARG:NH2 | 1:A:145:ARG:HE | 0.42 | 2.13 | 7 | 1 |
| 1:A:8:LEU:HG | 1:A:200:ASP:OD2 | 0.42 | 2.15 | 9 | 3 |
| 1:A:57:LYS:CD | 1:A:100:ILE:O | 0.42 | 2.68 | 13 | 1 |
| 1:A:62:PRO:O | 1:A:95:TYR:CD2 | 0.42 | 2.73 | 2 | 3 |
| 1:A:127:VAL:HB | 1:A:142:ARG:HE | 0.42 | 1.75 | 16 | 1 |
| 1:A:123:VAL:O | 1:A:124:GLY:C | 0.42 | 2.57 | 12 | 3 |
| 1:A:171:GLU:O | 1:A:172:ALA:C | 0.42 | 2.57 | 14 | 2 |
| 1:A:128:ASP:HB2 | 1:A:142:ARG:NE | 0.42 | 2.30 | 19 | 1 |
| 1:A:145:ARG:CZ | 1:A:149:GLU:OE2 | 0.42 | 2.68 | 18 | 1 |
| 1:A:145:ARG:HG2 | 1:A:149:GLU:OE1 | 0.42 | 2.15 | 11 | 3 |
| 1:A:38:PHE:CE2 | 1:A:79:TYR:HE1 | 0.42 | 2.33 | 13 | 1 |
| 1:A:58:TYR:CD1 | 1:A:58:TYR:O | 0.42 | 2.72 | 16 | 1 |
| 1:A:24:LEU:HD12 | 1:A:118:GLU:CA | 0.42 | 2.45 | 11 | 1 |
| 1:A:128:ASP:OD1 | 1:A:142:ARG:HG3 | 0.42 | 2.15 | 2 | 1 |
| 1:A:145:ARG:HG3 | 1:A:149:GLU:OE2 | 0.41 | 2.14 | 6 | 2 |
| 1:A:143:VAL:HG12 | 1:A:147:LEU:HD11 | 0.41 | 1.91 | 15 | 1 |
| 1:A:161:ASN:O | 1:A:162:ARG:C | 0.41 | 2.56 | 10 | 3 |
| 1:A:87:PHE:CZ | 1:A:89:ALA:CA | 0.41 | 3.03 | 20 | 1 |
| 1:A:69:TYR:CD2 | 1:A:150:ASN:OD1 | 0.41 | 2.73 | 20 | 1 |
| 1:A:56:MET:HE2 | 1:A:56:MET:HB3 | 0.41 | 1.63 | 7 | 1 |
| 1:A:138:ALA:O | 1:A:187:GLN:OE1 | 0.41 | 2.38 | 11 | 1 |
| 1:A:44:ALA:HB3 | 1:A:135:SER:HB2 | 0.41 | 1.92 | 6 | 1 |
| 1:A:6:SER:HB3 | 1:A:9:ASP:HB2 | 0.41 | 1.91 | 6 | 3 |
| 1:A:157:VAL:HG23 | 1:A:250:GLY:O | 0.41 | 2.16 | 18 | 1 |
| 1:A:177:GLU:OE1 | 1:A:250:GLY:HA2 | 0.41 | 2.14 | 13 | 1 |
| 1:A:93:ARG:HD2 | 1:A:122:ASP:OD2 | 0.41 | 2.15 | 9 | 3 |
| 1:A:31:VAL:HG22 | 1:A:37:SER:OG | 0.41 | 2.15 | 4 | 1 |
| 1:A:127:VAL:C | 1:A:142:ARG:HD2 | 0.41 | 2.35 | 16 | 1 |
| 1:A:146:ALA:O | 1:A:151:PHE:CD2 | 0.41 | 2.73 | 11 | 1 |
| 1:A:27:VAL:CG2 | 1:A:42:HIS:CE1 | 0.41 | 3.03 | 3 | 1 |
| 1:A:58:TYR:CD1 | 1:A:59:HIS:CE1 | 0.41 | 3.08 | 20 | 1 |
| 1:A:189:VAL:HA | 1:A:194:GLY:HA2 | 0.41 | 1.91 | 16 | 2 |
| 1:A:123:VAL:HA | 1:A:126:SER:OG | 0.41 | 2.15 | 7 | 2 |
| 1:A:67:LYS:HA | 1:A:91:SER:HB3 | 0.41 | 1.93 | 18 | 4 |
| 1:A:13:ILE:HG12 | 1:A:102:PRO:HB3 | 0.41 | 1.90 | 2 | 3 |
| 1:A:56:MET:HE1 | 1:A:151:PHE:CD1 | 0.41 | 2.50 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:54:GLN:O | 1:A:57:LYS:N | 0.41 | 2.53 | 4 | 1 |
| 1:A:145:ARG:HG3 | 1:A:149:GLU:CD | 0.41 | 2.36 | 11 | 1 |
| 1:A:187:GLN:CA | 1:A:196:ALA:HA | 0.41 | 2.46 | 3 | 1 |
| 1:A:19:ASN:HD22 | 1:A:19:ASN:N | 0.41 | 2.13 | 18 | 1 |
| 1:A:200:ASP:OD1 | 1:A:209:HIS:HB3 | 0.41 | 2.15 | 13 | 1 |
| 1:A:60:ASN:HB3 | 1:A:97:TRP:CD1 | 0.41 | 2.51 | 16 | 1 |
| 1:A:174:ILE:O | 1:A:177:GLU:HB2 | 0.41 | 2.15 | 4 | 3 |
| 1:A:116:ILE:CG2 | 1:A:117:SER:N | 0.41 | 2.83 | 18 | 2 |
| 1:A:144:GLN:C | 1:A:144:GLN:OE1 | 0.41 | 2.59 | 7 | 1 |
| 1:A:209:HIS:ND1 | 1:A:210:VAL:N | 0.41 | 2.69 | 17 | 1 |
| 1:A:86:LEU:N | 1:A:86:LEU:CD1 | 0.41 | 2.82 | 17 | 1 |
| 1:A:57:LYS:HD3 | 1:A:100:ILE:HG22 | 0.41 | 1.93 | 5 | 1 |
| 1:A:127:VAL:HB | 1:A:142:ARG:HH21 | 0.41 | 1.75 | 16 | 1 |
| 1:A:19:ASN:OD1 | 1:A:106:GLY:HA3 | 0.41 | 2.16 | 11 | 1 |
| 1:A:63:ASN:OD1 | 1:A:95:TYR:O | 0.41 | 2.39 | 11 | 1 |
| 1:A:84:LYS:HG3 | 1:A:84:LYS:O | 0.41 | 2.15 | 5 | 3 |
| 1:A:38:PHE:O | 1:A:41:GLN:HG3 | 0.41 | 2.16 | 10 | 2 |
| 1:A:96:ASN:OD1 | 1:A:96:ASN:C | 0.41 | 2.58 | 12 | 1 |
| 1:A:71:TYR:HB2 | 1:A:128:ASP:OD1 | 0.41 | 2.15 | 15 | 1 |
| 1:A:48:VAL:HG13 | 1:A:143:VAL:CG2 | 0.41 | 2.46 | 7 | 1 |
| 1:A:169:ASP:N | 1:A:169:ASP:OD1 | 0.41 | 2.53 | 4 | 1 |
| 1:A:56:MET:HB3 | 1:A:56:MET:HE2 | 0.41 | 1.67 | 8 | 2 |
| 1:A:84:LYS:O | 1:A:84:LYS:HG3 | 0.41 | 2.16 | 15 | 2 |
| 1:A:122:ASP:O | 1:A:126:SER:N | 0.41 | 2.43 | 14 | 1 |
| 1:A:30:LYS:HD2 | 1:A:80:PHE:C | 0.41 | 2.36 | 15 | 1 |
| 1:A:48:VAL:CB | 1:A:137:SER:HB3 | 0.41 | 2.46 | 3 | 2 |
| 1:A:154:ASN:OD1 | 1:A:156:SER:N | 0.41 | 2.45 | 19 | 2 |
| 1:A:50:THR:HA | 1:A:120:MET:HE2 | 0.41 | 1.92 | 19 | 1 |
| 1:A:158:HIS:ND1 | 1:A:249:VAL:O | 0.41 | 2.54 | 20 | 2 |
| 1:A:159:GLN:HA | 1:A:247:ALA:O | 0.41 | 2.16 | 20 | 1 |
| 1:A:154:ASN:N | 1:A:252:LYS:O | 0.41 | 2.50 | 18 | 1 |
| 1:A:7:LEU:HD12 | 1:A:183:PRO:N | 0.41 | 2.31 | 13 | 1 |
| 1:A:11:LYS:CB | 1:A:13:ILE:HG13 | 0.41 | 2.46 | 6 | 1 |
| 1:A:105:SER:OG | 1:A:108:GLU:OE1 | 0.41 | 2.39 | 6 | 1 |
| 1:A:24:LEU:HD23 | 1:A:24:LEU:HA | 0.41 | 1.77 | 1 | 1 |
| 1:A:48:VAL:HG11 | 1:A:137:SER:OG | 0.41 | 2.16 | 1 | 1 |
| 1:A:13:ILE:HG12 | 1:A:102:PRO:CB | 0.41 | 2.46 | 3 | 3 |
| 1:A:73:LEU:HD21 | 1:A:77:ASN:CG | 0.41 | 2.35 | 8 | 4 |
| 1:A:60:ASN:C | 1:A:97:TRP:CE2 | 0.41 | 2.94 | 12 | 1 |
| 1:A:15:TYR:HA | 1:A:21:TYR:CE2 | 0.41 | 2.50 | 12 | 2 |
| 1:A:68:ASP:CG | 1:A:91:SER:OG | 0.41 | 2.60 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:90:ILE:C | 1:A:92:THR:N | 0.41 | 2.73 | 16 | 3 |
| 1:A:21:TYR:N | 1:A:21:TYR:CD1 | 0.41 | 2.89 | 3 | 1 |
| 1:A:187:GLN:HB3 | 1:A:196:ALA:CB | 0.41 | 2.46 | 3 | 1 |
| 1:A:155:GLN:HA | 1:A:155:GLN:NE2 | 0.41 | 2.30 | 7 | 1 |
| 1:A:161:ASN:HA | 1:A:245:GLN:O | 0.41 | 2.16 | 13 | 1 |
| 1:A:162:ARG:O | 1:A:162:ARG:NE | 0.41 | 2.53 | 17 | 1 |
| 1:A:187:GLN:HE22 | 1:A:189:VAL:HG22 | 0.41 | 1.75 | 17 | 1 |
| 1:A:46:GLY:HA3 | 1:A:129:MET:HE1 | 0.41 | 1.93 | 10 | 1 |
| 1:A:38:PHE:CB | 1:A:41:GLN:NE2 | 0.41 | 2.83 | 4 | 1 |
| 1:A:201:GLY:O | 1:A:208:TYR:HB3 | 0.41 | 2.16 | 4 | 1 |
| 1:A:203:ASP:C | 1:A:205:ARG:N | 0.41 | 2.74 | 5 | 1 |
| 1:A:67:LYS:HG2 | 1:A:68:ASP:N | 0.41 | 2.30 | 11 | 1 |
| 1:A:69:TYR:CE2 | 1:A:70:THR:C | 0.41 | 2.94 | 1 | 1 |
| 1:A:140:SER:HB3 | 1:A:159:GLN:HG3 | 0.41 | 1.93 | 1 | 2 |
| 1:A:30:LYS:HD3 | 1:A:80:PHE:C | 0.41 | 2.36 | 8 | 1 |
| 1:A:174:ILE:HG21 | 1:A:199:ILE:HD12 | 0.41 | 1.91 | 12 | 1 |
| 1:A:122:ASP:O | 1:A:126:SER:CB | 0.41 | 2.69 | 14 | 1 |
| 1:A:173:GLN:HE21 | 1:A:249:VAL:HG21 | 0.41 | 1.76 | 7 | 1 |
| 1:A:104:TYR:OH | 1:A:116:ILE:HB | 0.41 | 2.16 | 17 | 1 |
| 1:A:148:LYS:HG3 | 1:A:157:VAL:HB | 0.41 | 1.93 | 17 | 1 |
| 1:A:252:LYS:O | 1:A:252:LYS:HG3 | 0.41 | 2.16 | 16 | 1 |
| 1:A:55:ILE:HD11 | 1:A:198:VAL:CG2 | 0.41 | 2.28 | 2 | 1 |
| 1:A:168:GLN:N | 1:A:168:GLN:CD | 0.40 | 2.73 | 8 | 1 |
| 1:A:99:ASN:O | 1:A:101:LEU:N | 0.40 | 2.54 | 3 | 1 |
| 1:A:104:TYR:CZ | 1:A:116:ILE:CG2 | 0.40 | 3.05 | 18 | 1 |
| 1:A:167:LYS:HE2 | 1:A:171:GLU:OE2 | 0.40 | 2.16 | 10 | 1 |
| 1:A:8:LEU:HB2 | 1:A:200:ASP:OD2 | 0.40 | 2.16 | 12 | 1 |
| 1:A:187:GLN:HB3 | 1:A:196:ALA:CA | 0.40 | 2.46 | 3 | 1 |
| 1:A:6:SER:HB3 | 1:A:209:HIS:ND1 | 0.40 | 2.32 | 19 | 1 |
| 1:A:71:TYR:CE1 | 1:A:86:LEU:CB | 0.40 | 3.02 | 20 | 1 |
| 1:A:60:ASN:ND2 | 1:A:97:TRP:HB3 | 0.40 | 2.32 | 18 | 1 |
| 1:A:168:GLN:N | 1:A:168:GLN:OE1 | 0.40 | 2.54 | 7 | 1 |
| 1:A:48:VAL:HA | 1:A:196:ALA:HB2 | 0.40 | 1.93 | 13 | 1 |
| 1:A:187:GLN:HG3 | 1:A:246:SER:O | 0.40 | 2.15 | 4 | 1 |
| 1:A:140:SER:HB3 | 1:A:159:GLN:CD | 0.40 | 2.36 | 5 | 1 |
| 1:A:46:GLY:HA2 | 1:A:135:SER:HB2 | 0.40 | 1.93 | 16 | 1 |
| 1:A:205:ARG:C | 1:A:207:PHE:N | 0.40 | 2.74 | 1 | 1 |
| 1:A:110:ASN:O | 1:A:114:MET:N | 0.40 | 2.44 | 8 | 1 |
| 1:A:24:LEU:HA | 1:A:24:LEU:HD23 | 0.40 | 1.78 | 15 | 1 |
| 1:A:179:SER:OG | 1:A:180:GLN:N | 0.40 | 2.55 | 13 | 1 |
| 1:A:71:TYR:CB | 1:A:128:ASP:OD2 | 0.40 | 2.69 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:99:ASN:HB3 | 1:A:115:ALA:HB2 | 0.40 | 1.93 | 20 | 1 |
| 1:A:197:PHE:HB3 | 1:A:212:TRP:HA | 0.40 | 1.92 | 18 | 1 |
| 1:A:139:GLY:O | 1:A:143:VAL:N | 0.40 | 2.38 | 7 | 1 |
| 1:A:68:ASP:OD1 | 1:A:91:SER:HB3 | 0.40 | 2.17 | 9 | 1 |
| 1:A:206:ASN:ND2 | 1:A:206:ASN:N | 0.40 | 2.69 | 9 | 1 |
| 1:A:172:ALA:O | 1:A:176:LYS:HB2 | 0.40 | 2.17 | 9 | 1 |
| 1:A:19:ASN:ND2 | 1:A:106:GLY:CA | 0.40 | 2.85 | 11 | 1 |
| 1:A:201:GLY:O | 1:A:208:TYR:HA | 0.40 | 2.16 | 2 | 1 |
| 1:A:138:ALA:CB | 1:A:142:ARG:NH2 | 0.40 | 2.82 | 1 | 1 |
| 1:A:23:LEU:HD11 | 1:A:113:LYS:NZ | 0.40 | 2.31 | 12 | 1 |
| 1:A:151:PHE:O | 1:A:153:TYR:N | 0.40 | 2.54 | 19 | 1 |
| 1:A:15:TYR:CD2 | 1:A:54:GLN:HG3 | 0.40 | 2.50 | 19 | 1 |
| 1:A:7:LEU:HD13 | 1:A:181:ASN:O | 0.40 | 2.16 | 19 | 1 |
| 1:A:21:TYR:CD1 | 1:A:116:ILE:HG12 | 0.40 | 2.51 | 18 | 1 |
| 1:A:20:PRO:HB3 | 1:A:113:LYS:CE | 0.40 | 2.46 | 13 | 1 |

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | | |
|-----|-------|-----------------|---------------|--------------|------------|-------------|----|--|
| 1 | A | 212/253 (84%) | 184±3 (87±1%) | 24±2 (11±1%) | 5±1 (2±0%) | 13 | 52 | |
| All | All | 4240/5060 (84%) | 3673 (87%) | 473 (11%) | 94 (2%) | 13 | 52 | |

All 7 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 | 81 | ASN | 20 |
| 1 | A | 19 | ASN | 20 |
| 1 | A | 82 | HIS | 20 |
| 1 | A | 212 | TRP | 18 |
| 1 | A | 61 | TYR | 10 |
| 1 | A | 152 | GLY | 5 |
| 1 | A | 206 | ASN | 1 |

6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|---------------|--------------|-------------|----|
| 1 | A | 179/204 (88%) | 156±4 (87±2%) | 23±4 (13±2%) | 9 | 51 |
| All | All | 3580/4080 (88%) | 3119 (87%) | 461 (13%) | 9 | 51 |

All 79 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 19 | ASN | 20 |
| 1 | A | 175 | ASP | 19 |
| 1 | A | 82 | HIS | 19 |
| 1 | A | 66 | LEU | 18 |
| 1 | A | 92 | THR | 18 |
| 1 | A | 185 | TYR | 17 |
| 1 | A | 252 | LYS | 15 |
| 1 | A | 109 | SER | 15 |
| 1 | A | 94 | GLN | 13 |
| 1 | A | 85 | ASN | 12 |
| 1 | A | 191 | LYS | 12 |
| 1 | A | 203 | ASP | 12 |
| 1 | A | 134 | SER | 12 |
| 1 | A | 112 | GLN | 11 |
| 1 | A | 74 | SER | 10 |
| 1 | A | 84 | LYS | 10 |
| 1 | A | 16 | ASN | 9 |
| 1 | A | 75 | SER | 9 |
| 1 | A | 60 | ASN | 9 |
| 1 | A | 103 | THR | 9 |
| 1 | A | 37 | SER | 8 |
| 1 | A | 206 | ASN | 8 |
| 1 | A | 76 | ASN | 7 |
| 1 | A | 108 | GLU | 7 |
| 1 | A | 50 | THR | 7 |
| 1 | A | 91 | SER | 7 |
| 1 | A | 187 | GLN | 7 |
| 1 | A | 70 | THR | 6 |
| 1 | A | 107 | ARG | 6 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 166 | SER | 5 |
| 1 | A | 126 | SER | 5 |
| 1 | A | 141 | SER | 5 |
| 1 | A | 68 | ASP | 5 |
| 1 | A | 64 | LYS | 5 |
| 1 | A | 145 | ARG | 5 |
| 1 | A | 162 | ARG | 5 |
| 1 | A | 93 | ARG | 4 |
| 1 | A | 98 | ASN | 4 |
| 1 | A | 9 | ASP | 4 |
| 1 | A | 205 | ARG | 4 |
| 1 | A | 168 | GLN | 4 |
| 1 | A | 130 | ASP | 4 |
| 1 | A | 114 | MET | 3 |
| 1 | A | 96 | ASN | 3 |
| 1 | A | 246 | SER | 3 |
| 1 | A | 10 | SER | 3 |
| 1 | A | 63 | ASN | 3 |
| 1 | A | 118 | GLU | 3 |
| 1 | A | 137 | SER | 3 |
| 1 | A | 169 | ASP | 3 |
| 1 | A | 42 | HIS | 3 |
| 1 | A | 120 | MET | 3 |
| 1 | A | 140 | SER | 2 |
| 1 | A | 158 | HIS | 2 |
| 1 | A | 207 | PHE | 2 |
| 1 | A | 144 | GLN | 2 |
| 1 | A | 164 | ASP | 2 |
| 1 | A | 110 | ASN | 2 |
| 1 | A | 105 | SER | 2 |
| 1 | A | 72 | THR | 2 |
| 1 | A | 135 | SER | 2 |
| 1 | A | 6 | SER | 2 |
| 1 | A | 80 | PHE | 2 |
| 1 | A | 11 | LYS | 2 |
| 1 | A | 128 | ASP | 2 |
| 1 | A | 209 | HIS | 1 |
| 1 | A | 212 | TRP | 1 |
| 1 | A | 176 | LYS | 1 |
| 1 | A | 245 | GLN | 1 |
| 1 | A | 30 | LYS | 1 |
| 1 | A | 142 | ARG | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 87 | PHE | 1 |
| 1 | A | 69 | TYR | 1 |
| 1 | A | 150 | ASN | 1 |
| 1 | A | 156 | SER | 1 |
| 1 | A | 179 | SER | 1 |
| 1 | A | 23 | LEU | 1 |
| 1 | A | 155 | GLN | 1 |
| 1 | A | 47 | SER | 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 carbohydrates 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

No chemical shift data were provided