



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 07:17 PM BST

PDB ID : 4V4M
Title : 1.45 Angstrom Structure of STNV coat protein
Authors : Lane, S.W.; Dennis, C.A.; Lane, C.L.; Trinh, C.H.; Rizkallah, P.J.; Stockley, P.G.; Phillips, S.E.V.
Deposited on : 2011-04-28
Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

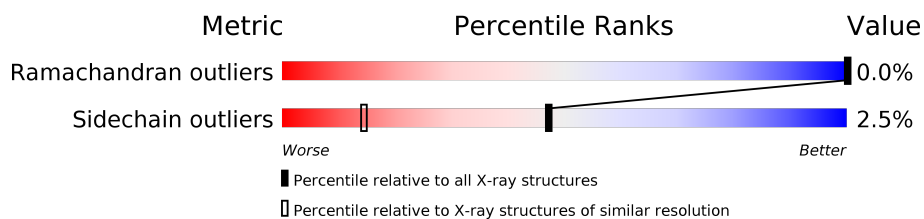
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Ramachandran outliers | 138981 | 1178 (1.46-1.46) |
| Sidechain outliers | 138945 | 1178 (1.46-1.46) |

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 307.58 Å 302.26 Å 181.92 Å 90.00° 92.77° 90.00° | Depositor |
| Resolution (Å) | 12.00 – 1.45 | Depositor |
| % Data completeness (in resolution range) | 99.9 (12.00-1.45) | Depositor |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.55 (at 1.45 Å) | Xtriage |
| Refinement program | REFMAC 5.5.0066 | Depositor |
| R, R_{free} | 0.175 , 0.208 | Depositor |
| Wilson B-factor (Å ²) | 10.1 | Xtriage |
| Anisotropy | 0.059 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.007 for k,h,-l 0.009 for -k,-h,-l 0.013 for -h,-k,l | Xtriage |
| Total number of atoms | 102135 | wwPDB-VP |
| Average B, all atoms (Å ²) | 15.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality ⓘ

3.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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 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 | 0 | 0.47 | 0/1468 | 0.64 | 1/1988 (0.1%) |
| 1 | 1 | 0.45 | 0/1477 | 0.64 | 1/2000 (0.1%) |
| 1 | 2 | 0.45 | 0/1486 | 0.62 | 0/2012 |
| 1 | 3 | 0.45 | 0/1488 | 0.63 | 1/2014 (0.0%) |
| 1 | 4 | 0.46 | 0/1474 | 0.62 | 1/1997 (0.1%) |
| 1 | 5 | 0.46 | 0/1457 | 0.61 | 0/1975 |
| 1 | 6 | 0.44 | 0/1479 | 0.62 | 1/2002 (0.0%) |
| 1 | 7 | 0.44 | 0/1466 | 0.62 | 0/1986 |
| 1 | A | 0.46 | 0/1500 | 0.65 | 0/2032 |
| 1 | B | 0.46 | 0/1504 | 0.63 | 0/2036 |
| 1 | C | 0.44 | 0/1485 | 0.61 | 0/2011 |
| 1 | D | 0.44 | 0/1479 | 0.64 | 2/2004 (0.1%) |
| 1 | E | 0.43 | 0/1465 | 0.62 | 0/1985 |
| 1 | F | 0.44 | 0/1466 | 0.62 | 0/1986 |
| 1 | G | 0.43 | 0/1484 | 0.62 | 0/2010 |
| 1 | H | 0.45 | 0/1468 | 0.61 | 0/1988 |
| 1 | I | 0.45 | 0/1474 | 0.62 | 0/1997 |
| 1 | J | 0.46 | 0/1468 | 0.64 | 0/1988 |
| 1 | K | 0.45 | 0/1513 | 0.67 | 0/2048 |
| 1 | L | 0.44 | 0/1495 | 0.60 | 1/2024 (0.0%) |
| 1 | M | 0.46 | 0/1473 | 0.61 | 0/1996 |
| 1 | N | 0.43 | 0/1476 | 0.63 | 1/1999 (0.1%) |
| 1 | O | 0.43 | 0/1468 | 0.61 | 0/1988 |
| 1 | P | 0.46 | 0/1505 | 0.62 | 0/2036 |
| 1 | Q | 0.45 | 0/1465 | 0.62 | 1/1985 (0.1%) |
| 1 | R | 0.46 | 0/1473 | 0.63 | 0/1996 |
| 1 | S | 0.47 | 0/1505 | 0.63 | 0/2037 |
| 1 | T | 0.47 | 0/1471 | 0.67 | 2/1993 (0.1%) |
| 1 | U | 0.46 | 0/1485 | 0.64 | 0/2011 |
| 1 | V | 0.47 | 0/1474 | 0.64 | 0/1997 |
| 1 | W | 0.44 | 0/1457 | 0.62 | 0/1974 |
| 1 | X | 0.46 | 0/1465 | 0.61 | 0/1985 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | Y | 0.47 | 0/1476 | 0.62 | 0/1999 |
| 1 | Z | 0.47 | 0/1479 | 0.65 | 0/2002 |
| 1 | a | 0.45 | 0/1493 | 0.64 | 0/2022 |
| 1 | b | 0.47 | 0/1457 | 0.65 | 1/1974 (0.1%) |
| 1 | c | 0.48 | 0/1479 | 0.62 | 0/2002 |
| 1 | d | 0.47 | 0/1464 | 0.64 | 1/1984 (0.1%) |
| 1 | e | 0.46 | 0/1464 | 0.64 | 0/1984 |
| 1 | f | 0.44 | 0/1484 | 0.61 | 0/2010 |
| 1 | g | 0.44 | 0/1465 | 0.62 | 0/1985 |
| 1 | h | 0.47 | 0/1485 | 0.65 | 0/2012 |
| 1 | i | 0.45 | 0/1476 | 0.61 | 0/1999 |
| 1 | j | 0.45 | 0/1469 | 0.63 | 0/1990 |
| 1 | k | 0.48 | 0/1468 | 0.64 | 0/1989 |
| 1 | l | 0.46 | 0/1457 | 0.64 | 1/1974 (0.1%) |
| 1 | m | 0.43 | 0/1468 | 0.60 | 0/1988 |
| 1 | n | 0.43 | 0/1484 | 0.62 | 0/2010 |
| 1 | o | 0.45 | 0/1458 | 0.62 | 0/1976 |
| 1 | p | 0.45 | 0/1457 | 0.64 | 1/1974 (0.1%) |
| 1 | q | 0.47 | 0/1457 | 0.64 | 1/1974 (0.1%) |
| 1 | r | 0.47 | 0/1479 | 0.65 | 1/2002 (0.0%) |
| 1 | s | 0.46 | 0/1464 | 0.63 | 0/1984 |
| 1 | t | 0.44 | 0/1515 | 0.62 | 1/2050 (0.0%) |
| 1 | u | 0.46 | 0/1468 | 0.61 | 0/1988 |
| 1 | v | 0.46 | 0/1468 | 0.64 | 0/1988 |
| 1 | w | 0.47 | 0/1475 | 0.65 | 0/1998 |
| 1 | x | 0.46 | 0/1476 | 0.63 | 0/1999 |
| 1 | y | 0.46 | 0/1464 | 0.64 | 0/1984 |
| 1 | z | 0.46 | 0/1485 | 0.64 | 2/2011 (0.1%) |
| All | All | 0.45 | 0/88547 | 0.63 | 21/119932 (0.0%) |

There are no bond length outliers.

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1 | l | 31 | LEU | CA-CB-CG | 6.64 | 130.58 | 115.30 |
| 1 | q | 31 | LEU | CA-CB-CG | 6.54 | 130.35 | 115.30 |
| 1 | p | 31 | LEU | CA-CB-CG | 6.10 | 129.32 | 115.30 |
| 1 | 4 | 31 | LEU | CA-CB-CG | 5.94 | 128.96 | 115.30 |
| 1 | 3 | 31 | LEU | CA-CB-CG | 5.89 | 128.85 | 115.30 |
| 1 | t | 31 | LEU | CA-CB-CG | 5.82 | 128.68 | 115.30 |
| 1 | 1 | 31 | LEU | CA-CB-CG | 5.75 | 128.52 | 115.30 |
| 1 | N | 31 | LEU | CA-CB-CG | 5.72 | 128.46 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-------|------|----------|------|-------------|----------|
| 1 | r | 31 | LEU | CA-CB-CG | 5.54 | 128.05 | 115.30 |
| 1 | D | 31[A] | LEU | CA-CB-CG | 5.49 | 127.93 | 115.30 |
| 1 | D | 31[B] | LEU | CA-CB-CG | 5.49 | 127.93 | 115.30 |
| 1 | 6 | 31 | LEU | CA-CB-CG | 5.37 | 127.65 | 115.30 |
| 1 | d | 31 | LEU | CA-CB-CG | 5.32 | 127.53 | 115.30 |
| 1 | T | 31[A] | LEU | CA-CB-CG | 5.31 | 127.52 | 115.30 |
| 1 | T | 31[B] | LEU | CA-CB-CG | 5.31 | 127.52 | 115.30 |
| 1 | 0 | 31 | LEU | CA-CB-CG | 5.30 | 127.50 | 115.30 |
| 1 | L | 31 | LEU | CA-CB-CG | 5.28 | 127.45 | 115.30 |
| 1 | Q | 31 | LEU | CA-CB-CG | 5.12 | 127.09 | 115.30 |
| 1 | z | 31[A] | LEU | CA-CB-CG | 5.10 | 127.03 | 115.30 |
| 1 | z | 31[B] | LEU | CA-CB-CG | 5.10 | 127.03 | 115.30 |
| 1 | b | 31 | LEU | CA-CB-CG | 5.09 | 127.00 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

3.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

3.3 Torsion angles [i](#)

3.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 0 | 184/196 (94%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 1 | 185/196 (94%) | 178 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | 2 | 186/196 (95%) | 180 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | 3 | 186/196 (95%) | 181 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 4 | 185/196 (94%) | 179 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | 5 | 183/196 (93%) | 179 (98%) | 4 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 6 | 185/196 (94%) | 180 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 7 | 184/196 (94%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | A | 188/196 (96%) | 183 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | B | 188/196 (96%) | 183 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | C | 186/196 (95%) | 181 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | D | 186/196 (95%) | 181 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | E | 184/196 (94%) | 176 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | F | 184/196 (94%) | 176 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | G | 186/196 (95%) | 178 (96%) | 7 (4%) | 1 (0%) | 29 | 9 |
| 1 | H | 184/196 (94%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | I | 185/196 (94%) | 180 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | J | 184/196 (94%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | K | 189/196 (96%) | 184 (97%) | 4 (2%) | 1 (0%) | 29 | 9 |
| 1 | L | 187/196 (95%) | 182 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | M | 185/196 (94%) | 178 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | N | 185/196 (94%) | 180 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | O | 184/196 (94%) | 180 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | P | 188/196 (96%) | 182 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | Q | 184/196 (94%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | R | 185/196 (94%) | 179 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | S | 188/196 (96%) | 182 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | T | 185/196 (94%) | 179 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | U | 186/196 (95%) | 181 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | V | 185/196 (94%) | 180 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | W | 183/196 (93%) | 176 (96%) | 6 (3%) | 1 (0%) | 29 | 9 |
| 1 | X | 184/196 (94%) | 180 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | Y | 185/196 (94%) | 180 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | Z | 185/196 (94%) | 179 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | a | 187/196 (95%) | 182 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | b | 183/196 (93%) | 179 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | c | 185/196 (94%) | 179 (97%) | 5 (3%) | 1 (0%) | 29 | 9 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1 | d | 184/196 (94%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | e | 184/196 (94%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | f | 186/196 (95%) | 178 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | g | 184/196 (94%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | h | 186/196 (95%) | 181 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | i | 185/196 (94%) | 179 (97%) | 5 (3%) | 1 (0%) | 29 | 9 |
| 1 | j | 184/196 (94%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | k | 184/196 (94%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | l | 183/196 (93%) | 178 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | m | 184/196 (94%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | n | 186/196 (95%) | 180 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | o | 183/196 (93%) | 178 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | p | 183/196 (93%) | 178 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | q | 183/196 (93%) | 178 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | r | 185/196 (94%) | 179 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | s | 184/196 (94%) | 177 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | t | 189/196 (96%) | 183 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | u | 184/196 (94%) | 180 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | v | 184/196 (94%) | 179 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | w | 185/196 (94%) | 181 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | x | 185/196 (94%) | 178 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | y | 184/196 (94%) | 178 (97%) | 6 (3%) | 0 | 100 | 100 |
| 1 | z | 186/196 (95%) | 181 (97%) | 5 (3%) | 0 | 100 | 100 |
| All | All | 11101/11760 (94%) | 10766 (97%) | 330 (3%) | 5 (0%) | 100 | 100 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | W | 15 | ALA |
| 1 | G | 14 | ARG |
| 1 | K | 13 | MET |
| 1 | i | 14 | ARG |
| 1 | c | 13 | MET |

3.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 0 | 159/167 (95%) | 157 (99%) | 2 (1%) | 69 | 40 |
| 1 | 1 | 160/167 (96%) | 157 (98%) | 3 (2%) | 57 | 23 |
| 1 | 2 | 161/167 (96%) | 156 (97%) | 5 (3%) | 40 | 9 |
| 1 | 3 | 161/167 (96%) | 157 (98%) | 4 (2%) | 47 | 14 |
| 1 | 4 | 160/167 (96%) | 156 (98%) | 4 (2%) | 47 | 14 |
| 1 | 5 | 158/167 (95%) | 154 (98%) | 4 (2%) | 47 | 14 |
| 1 | 6 | 160/167 (96%) | 158 (99%) | 2 (1%) | 69 | 40 |
| 1 | 7 | 159/167 (95%) | 155 (98%) | 4 (2%) | 47 | 14 |
| 1 | A | 163/167 (98%) | 160 (98%) | 3 (2%) | 59 | 26 |
| 1 | B | 163/167 (98%) | 159 (98%) | 4 (2%) | 47 | 14 |
| 1 | C | 161/167 (96%) | 152 (94%) | 9 (6%) | 21 | 1 |
| 1 | D | 161/167 (96%) | 153 (95%) | 8 (5%) | 24 | 2 |
| 1 | E | 159/167 (95%) | 155 (98%) | 4 (2%) | 47 | 14 |
| 1 | F | 159/167 (95%) | 156 (98%) | 3 (2%) | 57 | 23 |
| 1 | G | 161/167 (96%) | 156 (97%) | 5 (3%) | 40 | 9 |
| 1 | H | 159/167 (95%) | 153 (96%) | 6 (4%) | 33 | 5 |
| 1 | I | 160/167 (96%) | 158 (99%) | 2 (1%) | 69 | 40 |
| 1 | J | 159/167 (95%) | 154 (97%) | 5 (3%) | 40 | 9 |
| 1 | K | 164/167 (98%) | 159 (97%) | 5 (3%) | 41 | 9 |
| 1 | L | 162/167 (97%) | 157 (97%) | 5 (3%) | 40 | 9 |
| 1 | M | 160/167 (96%) | 155 (97%) | 5 (3%) | 40 | 9 |
| 1 | N | 160/167 (96%) | 157 (98%) | 3 (2%) | 57 | 23 |
| 1 | O | 159/167 (95%) | 154 (97%) | 5 (3%) | 40 | 9 |
| 1 | P | 163/167 (98%) | 159 (98%) | 4 (2%) | 47 | 14 |
| 1 | Q | 159/167 (95%) | 154 (97%) | 5 (3%) | 40 | 9 |
| 1 | R | 160/167 (96%) | 154 (96%) | 6 (4%) | 33 | 5 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | S | 163/167 (98%) | 159 (98%) | 4 (2%) | 47 | 14 |
| 1 | T | 160/167 (96%) | 153 (96%) | 7 (4%) | 28 | 3 |
| 1 | U | 161/167 (96%) | 158 (98%) | 3 (2%) | 57 | 23 |
| 1 | V | 160/167 (96%) | 157 (98%) | 3 (2%) | 57 | 23 |
| 1 | W | 158/167 (95%) | 155 (98%) | 3 (2%) | 57 | 23 |
| 1 | X | 159/167 (95%) | 155 (98%) | 4 (2%) | 47 | 14 |
| 1 | Y | 160/167 (96%) | 156 (98%) | 4 (2%) | 47 | 14 |
| 1 | Z | 160/167 (96%) | 157 (98%) | 3 (2%) | 57 | 23 |
| 1 | a | 162/167 (97%) | 161 (99%) | 1 (1%) | 86 | 69 |
| 1 | b | 158/167 (95%) | 153 (97%) | 5 (3%) | 39 | 8 |
| 1 | c | 160/167 (96%) | 156 (98%) | 4 (2%) | 47 | 14 |
| 1 | d | 159/167 (95%) | 155 (98%) | 4 (2%) | 47 | 14 |
| 1 | e | 159/167 (95%) | 156 (98%) | 3 (2%) | 57 | 23 |
| 1 | f | 161/167 (96%) | 156 (97%) | 5 (3%) | 40 | 9 |
| 1 | g | 159/167 (95%) | 156 (98%) | 3 (2%) | 57 | 23 |
| 1 | h | 161/167 (96%) | 158 (98%) | 3 (2%) | 57 | 23 |
| 1 | i | 160/167 (96%) | 157 (98%) | 3 (2%) | 57 | 23 |
| 1 | j | 159/167 (95%) | 157 (99%) | 2 (1%) | 69 | 40 |
| 1 | k | 159/167 (95%) | 156 (98%) | 3 (2%) | 57 | 23 |
| 1 | l | 158/167 (95%) | 154 (98%) | 4 (2%) | 47 | 14 |
| 1 | m | 159/167 (95%) | 155 (98%) | 4 (2%) | 47 | 14 |
| 1 | n | 161/167 (96%) | 158 (98%) | 3 (2%) | 57 | 23 |
| 1 | o | 158/167 (95%) | 155 (98%) | 3 (2%) | 57 | 23 |
| 1 | p | 158/167 (95%) | 154 (98%) | 4 (2%) | 47 | 14 |
| 1 | q | 158/167 (95%) | 154 (98%) | 4 (2%) | 47 | 14 |
| 1 | r | 160/167 (96%) | 152 (95%) | 8 (5%) | 24 | 2 |
| 1 | s | 159/167 (95%) | 154 (97%) | 5 (3%) | 40 | 9 |
| 1 | t | 164/167 (98%) | 159 (97%) | 5 (3%) | 41 | 9 |
| 1 | u | 159/167 (95%) | 154 (97%) | 5 (3%) | 40 | 9 |
| 1 | v | 159/167 (95%) | 155 (98%) | 4 (2%) | 47 | 14 |
| 1 | w | 160/167 (96%) | 158 (99%) | 2 (1%) | 69 | 40 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 1 | x | 160/167 (96%) | 157 (98%) | 3 (2%) | 57 | 23 |
| 1 | y | 159/167 (95%) | 156 (98%) | 3 (2%) | 57 | 23 |
| 1 | z | 161/167 (96%) | 156 (97%) | 5 (3%) | 40 | 9 |
| All | All | 9601/10020 (96%) | 9357 (98%) | 244 (2%) | 47 | 14 |

All (244) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | e | 33 | ASN |
| 1 | e | 70 | HIS |
| 1 | e | 145 | ARG |
| 1 | f | 12 | THR |
| 1 | f | 28 | ARG |
| 1 | f | 33 | ASN |
| 1 | f | 70 | HIS |
| 1 | f | 73 | HIS |
| 1 | g | 33 | ASN |
| 1 | g | 70 | HIS |
| 1 | g | 73 | HIS |
| 1 | h | 33 | ASN |
| 1 | h | 70 | HIS |
| 1 | h | 73 | HIS |
| 1 | i | 33 | ASN |
| 1 | i | 70 | HIS |
| 1 | i | 73 | HIS |
| 1 | j | 70 | HIS |
| 1 | j | 73 | HIS |
| 1 | k | 31 | LEU |
| 1 | k | 33 | ASN |
| 1 | k | 70 | HIS |
| 1 | l | 31 | LEU |
| 1 | l | 33 | ASN |
| 1 | l | 70 | HIS |
| 1 | l | 73 | HIS |
| 1 | m | 22 | THR |
| 1 | m | 31 | LEU |
| 1 | m | 33 | ASN |
| 1 | m | 70 | HIS |
| 1 | n | 21 | ASN |
| 1 | n | 22 | THR |
| 1 | n | 70 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | o | 16 | VAL |
| 1 | o | 70 | HIS |
| 1 | o | 73 | HIS |
| 1 | p | 13 | MET |
| 1 | p | 31 | LEU |
| 1 | p | 33 | ASN |
| 1 | p | 70 | HIS |
| 1 | q | 16 | VAL |
| 1 | q | 28 | ARG |
| 1 | q | 31 | LEU |
| 1 | q | 70 | HIS |
| 1 | r | 12 | THR |
| 1 | r | 16 | VAL |
| 1 | r | 31 | LEU |
| 1 | r | 33 | ASN |
| 1 | r | 70 | HIS |
| 1 | r | 73 | HIS |
| 1 | r | 145[A] | ARG |
| 1 | r | 145[B] | ARG |
| 1 | s | 31 | LEU |
| 1 | s | 33 | ASN |
| 1 | s | 70 | HIS |
| 1 | s | 181[A] | VAL |
| 1 | s | 181[B] | VAL |
| 1 | t | 22 | THR |
| 1 | t | 31 | LEU |
| 1 | t | 33 | ASN |
| 1 | t | 70 | HIS |
| 1 | t | 73 | HIS |
| 1 | u | 16 | VAL |
| 1 | u | 31 | LEU |
| 1 | u | 33 | ASN |
| 1 | u | 70 | HIS |
| 1 | u | 73 | HIS |
| 1 | v | 13 | MET |
| 1 | v | 31 | LEU |
| 1 | v | 70 | HIS |
| 1 | v | 73 | HIS |
| 1 | w | 70 | HIS |
| 1 | w | 73 | HIS |
| 1 | x | 66 | ARG |
| 1 | x | 70 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 1 | x | 73 | HIS |
| 1 | y | 16 | VAL |
| 1 | y | 70 | HIS |
| 1 | y | 73 | HIS |
| 1 | z | 22 | THR |
| 1 | z | 31[A] | LEU |
| 1 | z | 31[B] | LEU |
| 1 | z | 33 | ASN |
| 1 | z | 70 | HIS |
| 1 | 0 | 31 | LEU |
| 1 | 0 | 70 | HIS |
| 1 | 1 | 31 | LEU |
| 1 | 1 | 33 | ASN |
| 1 | 1 | 70 | HIS |
| 1 | 2 | 16 | VAL |
| 1 | 2 | 31 | LEU |
| 1 | 2 | 33 | ASN |
| 1 | 2 | 70 | HIS |
| 1 | 2 | 73 | HIS |
| 1 | 3 | 31 | LEU |
| 1 | 3 | 33 | ASN |
| 1 | 3 | 70 | HIS |
| 1 | 3 | 73 | HIS |
| 1 | 4 | 31 | LEU |
| 1 | 4 | 33 | ASN |
| 1 | 4 | 70 | HIS |
| 1 | 4 | 73 | HIS |
| 1 | 5 | 16 | VAL |
| 1 | 5 | 33 | ASN |
| 1 | 5 | 70 | HIS |
| 1 | 5 | 73 | HIS |
| 1 | 6 | 31 | LEU |
| 1 | 6 | 70 | HIS |
| 1 | 7 | 33 | ASN |
| 1 | 7 | 70 | HIS |
| 1 | 7 | 71 | LYS |
| 1 | 7 | 73 | HIS |
| 1 | A | 22 | THR |
| 1 | A | 33 | ASN |
| 1 | A | 70 | HIS |
| 1 | B | 33 | ASN |
| 1 | B | 70 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | B | 146[A] | ILE |
| 1 | B | 146[B] | ILE |
| 1 | C | 18 | ARG |
| 1 | C | 22 | THR |
| 1 | C | 31 | LEU |
| 1 | C | 33 | ASN |
| 1 | C | 70 | HIS |
| 1 | C | 73 | HIS |
| 1 | C | 129 | LYS |
| 1 | C | 148[A] | ASN |
| 1 | C | 148[B] | ASN |
| 1 | D | 13 | MET |
| 1 | D | 16 | VAL |
| 1 | D | 31[A] | LEU |
| 1 | D | 31[B] | LEU |
| 1 | D | 34[A] | SER |
| 1 | D | 34[B] | SER |
| 1 | D | 70 | HIS |
| 1 | D | 129 | LYS |
| 1 | E | 12 | THR |
| 1 | E | 33 | ASN |
| 1 | E | 70 | HIS |
| 1 | E | 73 | HIS |
| 1 | F | 33 | ASN |
| 1 | F | 70 | HIS |
| 1 | F | 73 | HIS |
| 1 | G | 16 | VAL |
| 1 | G | 33 | ASN |
| 1 | G | 70 | HIS |
| 1 | G | 73 | HIS |
| 1 | G | 129 | LYS |
| 1 | H | 14 | ARG |
| 1 | H | 16 | VAL |
| 1 | H | 33 | ASN |
| 1 | H | 70 | HIS |
| 1 | H | 91[A] | ARG |
| 1 | H | 91[B] | ARG |
| 1 | I | 22 | THR |
| 1 | I | 70 | HIS |
| 1 | J | 12 | THR |
| 1 | J | 13 | MET |
| 1 | J | 16 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | J | 33 | ASN |
| 1 | J | 70 | HIS |
| 1 | K | 16 | VAL |
| 1 | K | 33 | ASN |
| 1 | K | 70 | HIS |
| 1 | K | 73 | HIS |
| 1 | K | 95 | ASN |
| 1 | L | 19 | MET |
| 1 | L | 31 | LEU |
| 1 | L | 33 | ASN |
| 1 | L | 70 | HIS |
| 1 | L | 73 | HIS |
| 1 | M | 17 | LYS |
| 1 | M | 33 | ASN |
| 1 | M | 70 | HIS |
| 1 | M | 73 | HIS |
| 1 | M | 129 | LYS |
| 1 | N | 31 | LEU |
| 1 | N | 70 | HIS |
| 1 | N | 73 | HIS |
| 1 | O | 12 | THR |
| 1 | O | 31 | LEU |
| 1 | O | 70 | HIS |
| 1 | O | 73 | HIS |
| 1 | O | 129 | LYS |
| 1 | P | 31 | LEU |
| 1 | P | 33 | ASN |
| 1 | P | 70 | HIS |
| 1 | P | 73 | HIS |
| 1 | Q | 31 | LEU |
| 1 | Q | 70 | HIS |
| 1 | Q | 73 | HIS |
| 1 | Q | 148[A] | ASN |
| 1 | Q | 148[B] | ASN |
| 1 | R | 16 | VAL |
| 1 | R | 31[A] | LEU |
| 1 | R | 31[B] | LEU |
| 1 | R | 33 | ASN |
| 1 | R | 70 | HIS |
| 1 | R | 71 | LYS |
| 1 | S | 33 | ASN |
| 1 | S | 70 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | S | 152[A] | GLN |
| 1 | S | 152[B] | GLN |
| 1 | T | 18 | ARG |
| 1 | T | 31[A] | LEU |
| 1 | T | 31[B] | LEU |
| 1 | T | 33 | ASN |
| 1 | T | 70 | HIS |
| 1 | T | 71 | LYS |
| 1 | T | 73 | HIS |
| 1 | U | 33 | ASN |
| 1 | U | 70 | HIS |
| 1 | U | 73 | HIS |
| 1 | V | 33 | ASN |
| 1 | V | 70 | HIS |
| 1 | V | 73 | HIS |
| 1 | W | 33 | ASN |
| 1 | W | 70 | HIS |
| 1 | W | 73 | HIS |
| 1 | X | 33 | ASN |
| 1 | X | 70 | HIS |
| 1 | X | 71 | LYS |
| 1 | X | 73 | HIS |
| 1 | Y | 31 | LEU |
| 1 | Y | 33 | ASN |
| 1 | Y | 70 | HIS |
| 1 | Y | 73 | HIS |
| 1 | Z | 33 | ASN |
| 1 | Z | 70 | HIS |
| 1 | Z | 73 | HIS |
| 1 | a | 70 | HIS |
| 1 | b | 12 | THR |
| 1 | b | 31 | LEU |
| 1 | b | 33 | ASN |
| 1 | b | 66 | ARG |
| 1 | b | 70 | HIS |
| 1 | c | 16 | VAL |
| 1 | c | 31 | LEU |
| 1 | c | 70 | HIS |
| 1 | c | 73 | HIS |
| 1 | d | 16 | VAL |
| 1 | d | 31 | LEU |
| 1 | d | 70 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | d | 145 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (487) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | e | 21 | ASN |
| 1 | e | 23 | HIS |
| 1 | e | 26 | HIS |
| 1 | e | 33 | ASN |
| 1 | e | 36 | ASN |
| 1 | e | 73 | HIS |
| 1 | e | 93 | ASN |
| 1 | e | 95 | ASN |
| 1 | e | 134 | ASN |
| 1 | f | 23 | HIS |
| 1 | f | 26 | HIS |
| 1 | f | 33 | ASN |
| 1 | f | 36 | ASN |
| 1 | f | 73 | HIS |
| 1 | f | 93 | ASN |
| 1 | f | 95 | ASN |
| 1 | f | 134 | ASN |
| 1 | g | 23 | HIS |
| 1 | g | 26 | HIS |
| 1 | g | 33 | ASN |
| 1 | g | 36 | ASN |
| 1 | g | 73 | HIS |
| 1 | g | 93 | ASN |
| 1 | g | 95 | ASN |
| 1 | g | 134 | ASN |
| 1 | g | 152 | GLN |
| 1 | h | 23 | HIS |
| 1 | h | 26 | HIS |
| 1 | h | 73 | HIS |
| 1 | h | 93 | ASN |
| 1 | h | 95 | ASN |
| 1 | h | 134 | ASN |
| 1 | i | 23 | HIS |
| 1 | i | 26 | HIS |
| 1 | i | 33 | ASN |
| 1 | i | 36 | ASN |
| 1 | i | 73 | HIS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | i | 93 | ASN |
| 1 | i | 95 | ASN |
| 1 | i | 134 | ASN |
| 1 | j | 23 | HIS |
| 1 | j | 26 | HIS |
| 1 | j | 33 | ASN |
| 1 | j | 73 | HIS |
| 1 | j | 93 | ASN |
| 1 | j | 95 | ASN |
| 1 | j | 134 | ASN |
| 1 | k | 26 | HIS |
| 1 | k | 33 | ASN |
| 1 | k | 36 | ASN |
| 1 | k | 73 | HIS |
| 1 | k | 93 | ASN |
| 1 | k | 95 | ASN |
| 1 | k | 134 | ASN |
| 1 | l | 26 | HIS |
| 1 | l | 33 | ASN |
| 1 | l | 36 | ASN |
| 1 | l | 45 | GLN |
| 1 | l | 73 | HIS |
| 1 | l | 93 | ASN |
| 1 | l | 95 | ASN |
| 1 | l | 134 | ASN |
| 1 | m | 21 | ASN |
| 1 | m | 26 | HIS |
| 1 | m | 33 | ASN |
| 1 | m | 36 | ASN |
| 1 | m | 73 | HIS |
| 1 | m | 93 | ASN |
| 1 | m | 95 | ASN |
| 1 | m | 134 | ASN |
| 1 | n | 21 | ASN |
| 1 | n | 23 | HIS |
| 1 | n | 26 | HIS |
| 1 | n | 33 | ASN |
| 1 | n | 36 | ASN |
| 1 | n | 73 | HIS |
| 1 | n | 93 | ASN |
| 1 | n | 95 | ASN |
| 1 | n | 134 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | o | 21 | ASN |
| 1 | o | 23 | HIS |
| 1 | o | 26 | HIS |
| 1 | o | 73 | HIS |
| 1 | o | 93 | ASN |
| 1 | o | 95 | ASN |
| 1 | o | 134 | ASN |
| 1 | p | 21 | ASN |
| 1 | p | 23 | HIS |
| 1 | p | 26 | HIS |
| 1 | p | 33 | ASN |
| 1 | p | 36 | ASN |
| 1 | p | 73 | HIS |
| 1 | p | 93 | ASN |
| 1 | p | 95 | ASN |
| 1 | p | 134 | ASN |
| 1 | q | 21 | ASN |
| 1 | q | 23 | HIS |
| 1 | q | 26 | HIS |
| 1 | q | 33 | ASN |
| 1 | q | 36 | ASN |
| 1 | q | 73 | HIS |
| 1 | q | 93 | ASN |
| 1 | q | 95 | ASN |
| 1 | q | 134 | ASN |
| 1 | q | 175 | GLN |
| 1 | r | 21 | ASN |
| 1 | r | 23 | HIS |
| 1 | r | 26 | HIS |
| 1 | r | 33 | ASN |
| 1 | r | 36 | ASN |
| 1 | r | 73 | HIS |
| 1 | r | 93 | ASN |
| 1 | r | 95 | ASN |
| 1 | r | 134 | ASN |
| 1 | s | 23 | HIS |
| 1 | s | 26 | HIS |
| 1 | s | 33 | ASN |
| 1 | s | 36 | ASN |
| 1 | s | 73 | HIS |
| 1 | s | 93 | ASN |
| 1 | s | 95 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | s | 134 | ASN |
| 1 | t | 21 | ASN |
| 1 | t | 23 | HIS |
| 1 | t | 26 | HIS |
| 1 | t | 33 | ASN |
| 1 | t | 36 | ASN |
| 1 | t | 45 | GLN |
| 1 | t | 73 | HIS |
| 1 | t | 93 | ASN |
| 1 | t | 95 | ASN |
| 1 | t | 134 | ASN |
| 1 | u | 21 | ASN |
| 1 | u | 23 | HIS |
| 1 | u | 26 | HIS |
| 1 | u | 33 | ASN |
| 1 | u | 36 | ASN |
| 1 | u | 73 | HIS |
| 1 | u | 93 | ASN |
| 1 | u | 95 | ASN |
| 1 | u | 134 | ASN |
| 1 | v | 26 | HIS |
| 1 | v | 33 | ASN |
| 1 | v | 36 | ASN |
| 1 | v | 73 | HIS |
| 1 | v | 93 | ASN |
| 1 | v | 95 | ASN |
| 1 | v | 134 | ASN |
| 1 | w | 23 | HIS |
| 1 | w | 26 | HIS |
| 1 | w | 33 | ASN |
| 1 | w | 36 | ASN |
| 1 | w | 73 | HIS |
| 1 | w | 93 | ASN |
| 1 | w | 95 | ASN |
| 1 | w | 134 | ASN |
| 1 | x | 23 | HIS |
| 1 | x | 26 | HIS |
| 1 | x | 33 | ASN |
| 1 | x | 36 | ASN |
| 1 | x | 73 | HIS |
| 1 | x | 93 | ASN |
| 1 | x | 95 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | x | 134 | ASN |
| 1 | x | 152 | GLN |
| 1 | y | 21 | ASN |
| 1 | y | 23 | HIS |
| 1 | y | 26 | HIS |
| 1 | y | 33 | ASN |
| 1 | y | 36 | ASN |
| 1 | y | 73 | HIS |
| 1 | y | 93 | ASN |
| 1 | y | 95 | ASN |
| 1 | y | 134 | ASN |
| 1 | z | 21 | ASN |
| 1 | z | 26 | HIS |
| 1 | z | 33 | ASN |
| 1 | z | 36 | ASN |
| 1 | z | 73 | HIS |
| 1 | z | 93 | ASN |
| 1 | z | 95 | ASN |
| 1 | z | 134 | ASN |
| 1 | 0 | 23 | HIS |
| 1 | 0 | 26 | HIS |
| 1 | 0 | 33 | ASN |
| 1 | 0 | 36 | ASN |
| 1 | 0 | 73 | HIS |
| 1 | 0 | 93 | ASN |
| 1 | 0 | 95 | ASN |
| 1 | 0 | 134 | ASN |
| 1 | 1 | 21 | ASN |
| 1 | 1 | 26 | HIS |
| 1 | 1 | 33 | ASN |
| 1 | 1 | 36 | ASN |
| 1 | 1 | 73 | HIS |
| 1 | 1 | 93 | ASN |
| 1 | 1 | 95 | ASN |
| 1 | 1 | 134 | ASN |
| 1 | 2 | 21 | ASN |
| 1 | 2 | 26 | HIS |
| 1 | 2 | 33 | ASN |
| 1 | 2 | 36 | ASN |
| 1 | 2 | 73 | HIS |
| 1 | 2 | 93 | ASN |
| 1 | 2 | 95 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 134 | ASN |
| 1 | 3 | 23 | HIS |
| 1 | 3 | 26 | HIS |
| 1 | 3 | 73 | HIS |
| 1 | 3 | 93 | ASN |
| 1 | 3 | 95 | ASN |
| 1 | 3 | 134 | ASN |
| 1 | 4 | 23 | HIS |
| 1 | 4 | 26 | HIS |
| 1 | 4 | 33 | ASN |
| 1 | 4 | 36 | ASN |
| 1 | 4 | 73 | HIS |
| 1 | 4 | 93 | ASN |
| 1 | 4 | 95 | ASN |
| 1 | 4 | 134 | ASN |
| 1 | 5 | 23 | HIS |
| 1 | 5 | 26 | HIS |
| 1 | 5 | 33 | ASN |
| 1 | 5 | 36 | ASN |
| 1 | 5 | 73 | HIS |
| 1 | 5 | 93 | ASN |
| 1 | 5 | 95 | ASN |
| 1 | 5 | 134 | ASN |
| 1 | 6 | 21 | ASN |
| 1 | 6 | 23 | HIS |
| 1 | 6 | 26 | HIS |
| 1 | 6 | 33 | ASN |
| 1 | 6 | 36 | ASN |
| 1 | 6 | 73 | HIS |
| 1 | 6 | 93 | ASN |
| 1 | 6 | 95 | ASN |
| 1 | 6 | 134 | ASN |
| 1 | 7 | 26 | HIS |
| 1 | 7 | 33 | ASN |
| 1 | 7 | 73 | HIS |
| 1 | 7 | 93 | ASN |
| 1 | 7 | 95 | ASN |
| 1 | 7 | 134 | ASN |
| 1 | A | 21 | ASN |
| 1 | A | 26 | HIS |
| 1 | A | 33 | ASN |
| 1 | A | 36 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 73 | HIS |
| 1 | A | 93 | ASN |
| 1 | A | 95 | ASN |
| 1 | A | 134 | ASN |
| 1 | B | 21 | ASN |
| 1 | B | 23 | HIS |
| 1 | B | 26 | HIS |
| 1 | B | 33 | ASN |
| 1 | B | 36 | ASN |
| 1 | B | 73 | HIS |
| 1 | B | 93 | ASN |
| 1 | B | 95 | ASN |
| 1 | B | 134 | ASN |
| 1 | C | 26 | HIS |
| 1 | C | 33 | ASN |
| 1 | C | 36 | ASN |
| 1 | C | 73 | HIS |
| 1 | C | 93 | ASN |
| 1 | C | 95 | ASN |
| 1 | C | 134 | ASN |
| 1 | D | 23 | HIS |
| 1 | D | 26 | HIS |
| 1 | D | 33 | ASN |
| 1 | D | 36 | ASN |
| 1 | D | 73 | HIS |
| 1 | D | 93 | ASN |
| 1 | D | 95 | ASN |
| 1 | D | 134 | ASN |
| 1 | E | 21 | ASN |
| 1 | E | 23 | HIS |
| 1 | E | 26 | HIS |
| 1 | E | 33 | ASN |
| 1 | E | 36 | ASN |
| 1 | E | 73 | HIS |
| 1 | E | 93 | ASN |
| 1 | E | 95 | ASN |
| 1 | E | 134 | ASN |
| 1 | F | 26 | HIS |
| 1 | F | 73 | HIS |
| 1 | F | 93 | ASN |
| 1 | F | 95 | ASN |
| 1 | F | 134 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 21 | ASN |
| 1 | G | 26 | HIS |
| 1 | G | 33 | ASN |
| 1 | G | 36 | ASN |
| 1 | G | 73 | HIS |
| 1 | G | 93 | ASN |
| 1 | G | 95 | ASN |
| 1 | G | 134 | ASN |
| 1 | H | 21 | ASN |
| 1 | H | 23 | HIS |
| 1 | H | 26 | HIS |
| 1 | H | 33 | ASN |
| 1 | H | 36 | ASN |
| 1 | H | 73 | HIS |
| 1 | H | 93 | ASN |
| 1 | H | 95 | ASN |
| 1 | H | 134 | ASN |
| 1 | I | 23 | HIS |
| 1 | I | 26 | HIS |
| 1 | I | 33 | ASN |
| 1 | I | 36 | ASN |
| 1 | I | 73 | HIS |
| 1 | I | 93 | ASN |
| 1 | I | 95 | ASN |
| 1 | I | 134 | ASN |
| 1 | J | 21 | ASN |
| 1 | J | 23 | HIS |
| 1 | J | 26 | HIS |
| 1 | J | 33 | ASN |
| 1 | J | 36 | ASN |
| 1 | J | 73 | HIS |
| 1 | J | 93 | ASN |
| 1 | J | 95 | ASN |
| 1 | J | 134 | ASN |
| 1 | K | 26 | HIS |
| 1 | K | 33 | ASN |
| 1 | K | 36 | ASN |
| 1 | K | 73 | HIS |
| 1 | K | 93 | ASN |
| 1 | K | 95 | ASN |
| 1 | K | 134 | ASN |
| 1 | L | 21 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 23 | HIS |
| 1 | L | 26 | HIS |
| 1 | L | 33 | ASN |
| 1 | L | 36 | ASN |
| 1 | L | 73 | HIS |
| 1 | L | 93 | ASN |
| 1 | L | 95 | ASN |
| 1 | L | 134 | ASN |
| 1 | M | 21 | ASN |
| 1 | M | 26 | HIS |
| 1 | M | 33 | ASN |
| 1 | M | 36 | ASN |
| 1 | M | 73 | HIS |
| 1 | M | 93 | ASN |
| 1 | M | 95 | ASN |
| 1 | M | 134 | ASN |
| 1 | N | 21 | ASN |
| 1 | N | 23 | HIS |
| 1 | N | 26 | HIS |
| 1 | N | 33 | ASN |
| 1 | N | 36 | ASN |
| 1 | N | 73 | HIS |
| 1 | N | 93 | ASN |
| 1 | N | 95 | ASN |
| 1 | N | 134 | ASN |
| 1 | N | 152 | GLN |
| 1 | O | 23 | HIS |
| 1 | O | 26 | HIS |
| 1 | O | 33 | ASN |
| 1 | O | 73 | HIS |
| 1 | O | 93 | ASN |
| 1 | O | 95 | ASN |
| 1 | O | 134 | ASN |
| 1 | P | 21 | ASN |
| 1 | P | 23 | HIS |
| 1 | P | 26 | HIS |
| 1 | P | 33 | ASN |
| 1 | P | 36 | ASN |
| 1 | P | 73 | HIS |
| 1 | P | 93 | ASN |
| 1 | P | 95 | ASN |
| 1 | P | 134 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 21 | ASN |
| 1 | Q | 23 | HIS |
| 1 | Q | 26 | HIS |
| 1 | Q | 33 | ASN |
| 1 | Q | 73 | HIS |
| 1 | Q | 93 | ASN |
| 1 | Q | 95 | ASN |
| 1 | Q | 134 | ASN |
| 1 | R | 21 | ASN |
| 1 | R | 26 | HIS |
| 1 | R | 33 | ASN |
| 1 | R | 36 | ASN |
| 1 | R | 73 | HIS |
| 1 | R | 93 | ASN |
| 1 | R | 95 | ASN |
| 1 | R | 134 | ASN |
| 1 | S | 23 | HIS |
| 1 | S | 26 | HIS |
| 1 | S | 33 | ASN |
| 1 | S | 36 | ASN |
| 1 | S | 73 | HIS |
| 1 | S | 93 | ASN |
| 1 | S | 95 | ASN |
| 1 | S | 134 | ASN |
| 1 | T | 23 | HIS |
| 1 | T | 26 | HIS |
| 1 | T | 33 | ASN |
| 1 | T | 73 | HIS |
| 1 | T | 93 | ASN |
| 1 | T | 95 | ASN |
| 1 | T | 134 | ASN |
| 1 | U | 23 | HIS |
| 1 | U | 26 | HIS |
| 1 | U | 33 | ASN |
| 1 | U | 36 | ASN |
| 1 | U | 73 | HIS |
| 1 | U | 93 | ASN |
| 1 | U | 95 | ASN |
| 1 | U | 134 | ASN |
| 1 | V | 23 | HIS |
| 1 | V | 26 | HIS |
| 1 | V | 33 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | V | 36 | ASN |
| 1 | V | 73 | HIS |
| 1 | V | 93 | ASN |
| 1 | V | 95 | ASN |
| 1 | V | 134 | ASN |
| 1 | W | 21 | ASN |
| 1 | W | 26 | HIS |
| 1 | W | 33 | ASN |
| 1 | W | 36 | ASN |
| 1 | W | 73 | HIS |
| 1 | W | 93 | ASN |
| 1 | W | 95 | ASN |
| 1 | W | 134 | ASN |
| 1 | X | 21 | ASN |
| 1 | X | 23 | HIS |
| 1 | X | 26 | HIS |
| 1 | X | 33 | ASN |
| 1 | X | 36 | ASN |
| 1 | X | 73 | HIS |
| 1 | X | 93 | ASN |
| 1 | X | 95 | ASN |
| 1 | X | 134 | ASN |
| 1 | Y | 26 | HIS |
| 1 | Y | 33 | ASN |
| 1 | Y | 36 | ASN |
| 1 | Y | 73 | HIS |
| 1 | Y | 93 | ASN |
| 1 | Y | 95 | ASN |
| 1 | Y | 134 | ASN |
| 1 | Z | 21 | ASN |
| 1 | Z | 26 | HIS |
| 1 | Z | 33 | ASN |
| 1 | Z | 36 | ASN |
| 1 | Z | 73 | HIS |
| 1 | Z | 93 | ASN |
| 1 | Z | 95 | ASN |
| 1 | Z | 134 | ASN |
| 1 | a | 23 | HIS |
| 1 | a | 26 | HIS |
| 1 | a | 33 | ASN |
| 1 | a | 36 | ASN |
| 1 | a | 73 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | a | 93 | ASN |
| 1 | a | 95 | ASN |
| 1 | a | 134 | ASN |
| 1 | b | 21 | ASN |
| 1 | b | 23 | HIS |
| 1 | b | 26 | HIS |
| 1 | b | 33 | ASN |
| 1 | b | 36 | ASN |
| 1 | b | 73 | HIS |
| 1 | b | 93 | ASN |
| 1 | b | 95 | ASN |
| 1 | b | 134 | ASN |
| 1 | b | 152 | GLN |
| 1 | c | 21 | ASN |
| 1 | c | 23 | HIS |
| 1 | c | 26 | HIS |
| 1 | c | 33 | ASN |
| 1 | c | 36 | ASN |
| 1 | c | 73 | HIS |
| 1 | c | 93 | ASN |
| 1 | c | 95 | ASN |
| 1 | c | 134 | ASN |
| 1 | d | 23 | HIS |
| 1 | d | 26 | HIS |
| 1 | d | 33 | ASN |
| 1 | d | 36 | ASN |
| 1 | d | 73 | HIS |
| 1 | d | 93 | ASN |
| 1 | d | 95 | ASN |
| 1 | d | 134 | ASN |

3.3.3 RNA ⓘ

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

3.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 92 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

4.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

4.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

4.4 Ligands

EDS failed to run properly - this section is therefore empty.

4.5 Other polymers

EDS failed to run properly - this section is therefore empty.