# Full wwPDB EM Validation Report

Apr 1, 2025 – 04:18 PM JST

| | | |
|---|---|---|
| PDB ID | : | 8KIA / pdb_00008kia |
| EMDB ID | : | EMD-37256 |
| Title | : | Tomato spotted wilt virus L protein (apo state) |
| Authors | : | Cao, L.; Wang, X. |
| Deposited on | : | 2023-08-23 |
| Resolution | : | 4.00 Å(reported) |

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

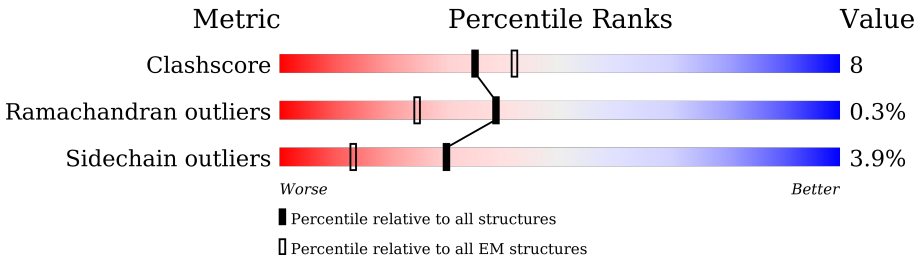
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev117 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.42 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1776 | 21% 68% 20% • 11% |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12717 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 1580 | 12717 | 8140 | 2090 | 2397 | 90 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

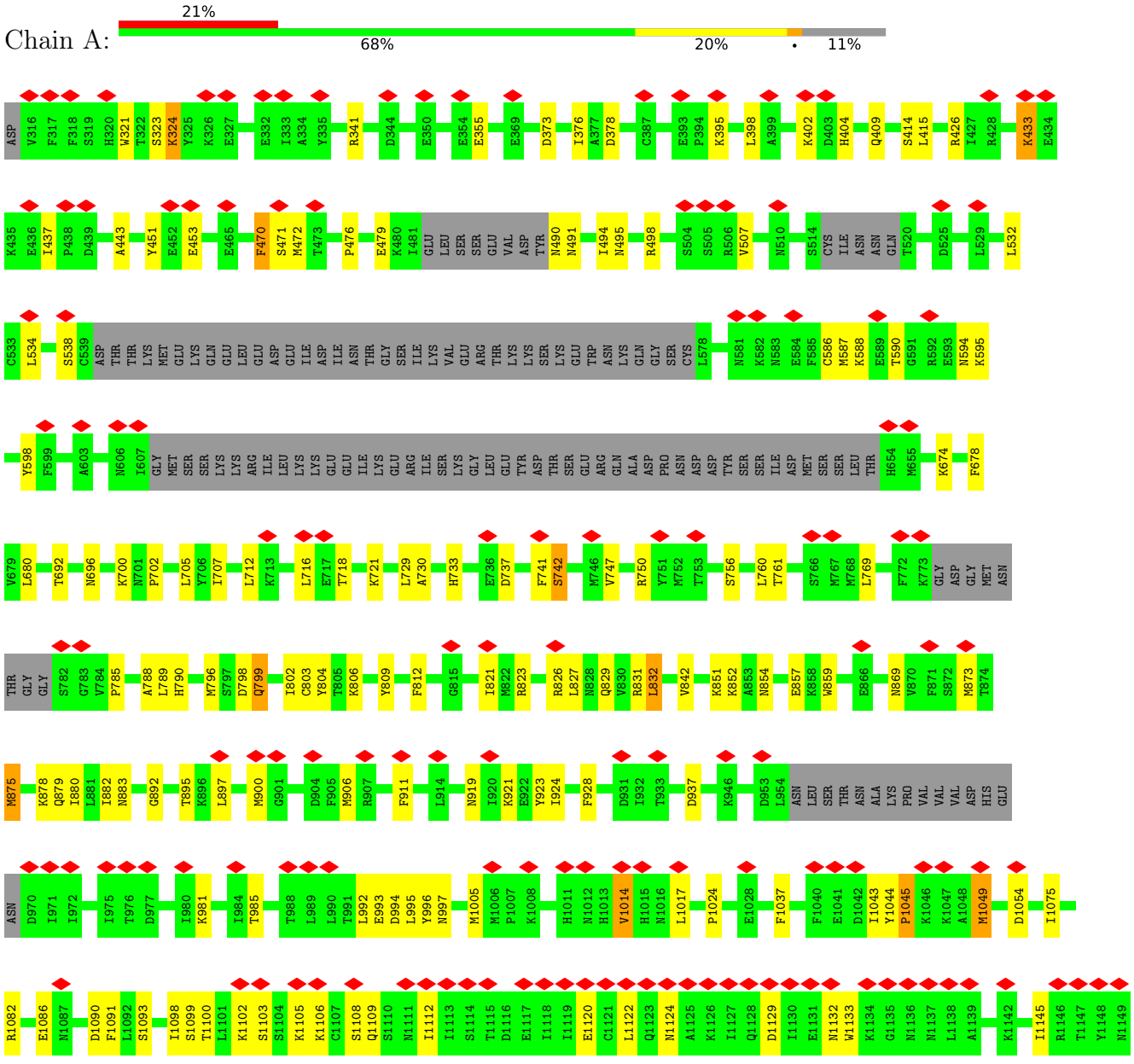
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 515 | CYS | SER | conflict | UNP A0A7G8JUQ9 |
| A | 1984 | GLY | CYS | conflict | UNP A0A7G8JUQ9 |

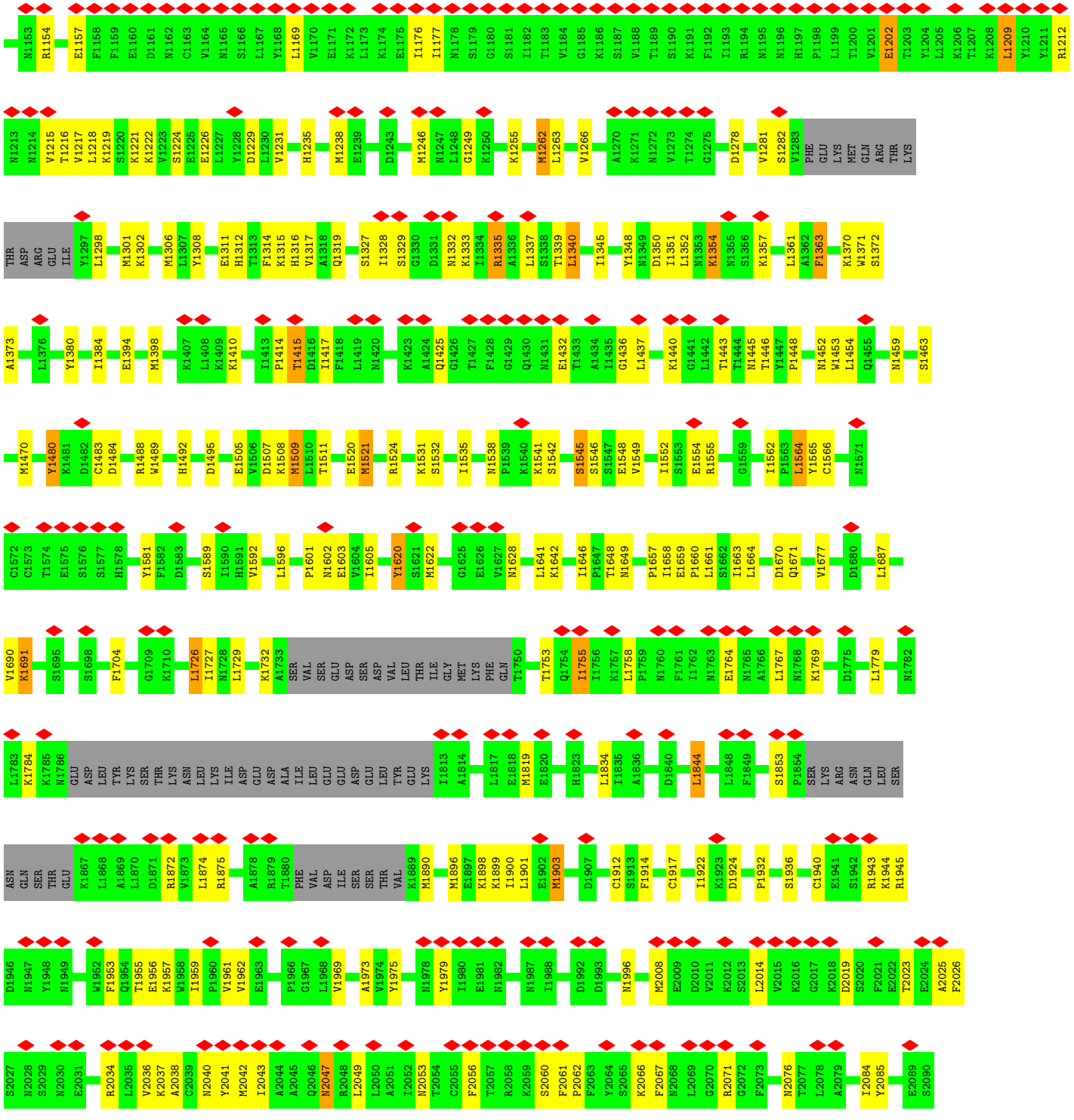
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA-directed RNA polymerase L

Chain A:




N1153 R1154 E1157 F1158 F1159 E1160 D1161 N1162 C1163 V1164 N1165 S1166 L1167 Y1168 L1169 V1170 E1171 K1172 L1173 K1174 E1175 I1176 I1177 N1178 S1179 G1180 S1181 I1182 T1183 V1184 G1185 K1186 S1187 V1188 T1189 S1190 K1191 F1192 I1193 R1194 N1195 N1196 H1197 P1198 L1199 T1200 V1201 E1202 T1203 Y1204 L1205 K1206 T1207 K1208 L1209 Y1210 Y1211 R1212
N1213 N1214 V1215 T1216 V1217 L1218 K1219 S1220 K1221 K1222 V1223 S1224 E1225 E1226 L1227 Y1228 D1229 L1230 V1231 H1235 M1238 E1239 D1243 M1246 N1247 L1248 G1249 K1250 K1255 M1262 L1263 V1266 A1270 K1271 N1272 V1273 T1274 G1275 D1278 V1281 S1282 V1283 PHE GLU LYS MET GLN ARG THR LYS
THR ASP ARG GLU ILE Y1297 L1298 M1301 K1302 M1306 L1307 Y1308 E1311 H1312 T1313 F1314 K1315 H1316 V1317 A1318 Q1319 S1327 I1328 S1329 G1330 D1331 N1332 K1333 I1334 R1335 A1336 L1337 S1338 T1339 L1340 I1345 Y1348 N1349 D1350 I1351 L1352 N1353 K1354 N1355 S1356 K1357 L1361 A1362 F1363 K1370 W1371 S1372
A1373 L1376 Y1380 I1384 E1394 M1398 K1407 L1408 K1409 K1410 I1413 P1414 T1415 D1416 I1417 F1418 L1419 N1420 K1423 A1424 Q1425 G1426 T1427 F1428 G1429 Q1430 N1431 E1432 T1433 A1434 I1435 G1436 L1437 K1440 G1441 L1442 T1443 T1444 N1445 T1446 Y1447 P1448 N1452 W1453 L1454 Q1455 N1459 S1463
M1470 Y1480 K1481 D1482 C1483 D1484 R1488 W1489 H1492 D1495 E1505 V1506 D1507 K1508 M1509 L1510 T1511 E1520 M1521 R1524 K1531 S1532 I1535 N1538 P1539 K1540 K1541 S1542 S1545 S1546 S1547 E1548 V1549 I1552 S1553 E1554 R1555 G1559 I1562 P1563 L1564 Y1565 C1566 N1571
C1572 C1573 T1574 E1575 S1576 S1577 H1578 Y1581 F1582 D1583 S1589 I1590 H1591 V1592 L1596 P1601 N1602 E1603 V1604 I1605 Y1620 S1621 M1622 G1625 E1626 V1627 N1628 L1641 K1642 I1646 P1647 T1648 N1649 P1657 I1658 E1659 P1660 L1661 S1662 I1663 L1664 D1670 Q1671 V1677 D1680 L1687
V1690 K1691 S1695 S1698 F1704 G1709 K1710 L1726 I1727 N1728 L1729 K1732 A1733 SER VAL SER GLU ASP SER ASP VAL LEU THR ILE GLY MET LYS PHE GLN T1750 T1753 Q1754 I1755 I1756 K1757 L1758 P1759 N1760 F1761 I1762 N1763 E1764 N1765 A1766 L1767 N1768 K1769 D1775 L1779 N1782
L1783 K1784 K1785 N1786 GLU ASP LEU TYR LYS SER THR LYS ASN LEU LYS ILE ASP GLU ASP ALA ILE LEU GLU GLU ASP GLU LEU TYR GLU LYS I1813 A1814 L1817 E1818 H1819 E1820 H1823 L1834 I1835 A1836 D1840 L1844 L1848 F1849 S1853 P1854 SER LYS ARG ASN GLN LEU SER
ASN GLN SER THR GLU K1867 L1868 A1869 L1870 D1871 R1872 V1873 L1874 R1875 A1878 R1879 T1880 PHE VAL ASP ILE SER SER THR VAL K1889 M1890 M1896 E1897 K1898 K1899 I1900 L1901 E1902 M1903 D1907 C1912 S1913 F1914 C1917 I1922 K1923 D1924 P1932 S1936 C1940 E1941 S1942 R1943 K1944 R1945
D1946 N1947 Y1948 N1949 W1952 F1953 Q1964 T1955 E1956 K1957 W1958 I1959 P1960 V1961 V1962 E1963 P1966 G1967 L1968 V1969 A1973 V1974 Y1975 N1978 Y1979 I1980 E1981 N1982 N1987 I1988 D1992 D1993 N1996 M2008 E2009 D2010 V2011 K2012 S2013 L2014 V2015 K2016 G2017 K2018 D2019 S2020 F2021 E2022 T2023 E2024 A2025 F2026
S2027 N2028 S2029 N2030 E2031 R2034 L2035 V2036 K2037 A2038 C2039 N2040 Y2041 M2042 I2043 A2044 A2045 Q2046 N2047 R2048 L2049 L2050 A2051 I2052 N2053 T2054 C2055 F2056 T2057 R2058 K2059 S2060 F2061 P2062 F2063 Y2064 S2065 K2066 F2067 N2068 L2069 G2070 R2071 G2072 F2073 N2076 T2077 L2078 A2079 I2084 Y2085 E2089 S2090

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 359068 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 60 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 1800 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 0.071 | Depositor |
| Minimum map value | -0.038 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.016 | Depositor |
| Map size (Å) | 374.4, 374.4, 374.4 | wwPDB |
| Map dimensions | 360, 360, 360 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.04, 1.04, 1.04 | Depositor |

# 5 Model quality

## 5.1 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 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 | 0.34 | 1/12952 (0.0%) | 0.73 | 31/17447 (0.2%) |

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 outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 859 | TRP | CB-CG | 5.46 | 1.60 | 1.50 |

All (31) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1209 | LEU | CA-CB-CG | 8.57 | 135.01 | 115.30 |
| 1 | A | 1340 | LEU | CA-CB-CG | 8.49 | 134.84 | 115.30 |
| 1 | A | 1509 | MET | CA-CB-CG | 7.73 | 126.44 | 113.30 |
| 1 | A | 1229 | ASP | CB-CG-OD1 | 7.70 | 125.23 | 118.30 |
| 1 | A | 1844 | LEU | CA-CB-CG | 7.32 | 132.13 | 115.30 |
| 1 | A | 1691 | LYS | CA-CB-CG | 6.41 | 127.49 | 113.40 |
| 1 | A | 1779 | LEU | CA-CB-CG | 6.33 | 129.85 | 115.30 |
| 1 | A | 1306 | MET | CA-CB-CG | 6.14 | 123.74 | 113.30 |
| 1 | A | 992 | LEU | CA-CB-CG | 6.09 | 129.31 | 115.30 |
| 1 | A | 1521 | MET | CA-CB-CG | 6.09 | 123.65 | 113.30 |
| 1 | A | 1361 | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 1 | A | 1890 | MET | CA-CB-CG | 5.98 | 123.47 | 113.30 |
| 1 | A | 1903 | MET | CA-CB-CG | 5.86 | 123.27 | 113.30 |
| 1 | A | 532 | LEU | CA-CB-CG | 5.68 | 128.36 | 115.30 |
| 1 | A | 1758 | LEU | CA-CB-CG | 5.67 | 128.35 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1202 | GLU | CA-CB-CG | 5.64 | 125.81 | 113.40 |
| 1 | A | 1437 | LEU | CA-CB-CG | 5.62 | 128.23 | 115.30 |
| 1 | A | 1263 | LEU | CA-CB-CG | 5.52 | 128.00 | 115.30 |
| 1 | A | 433 | LYS | CA-CB-CG | 5.48 | 125.45 | 113.40 |
| 1 | A | 1874 | LEU | CA-CB-CG | 5.42 | 127.76 | 115.30 |
| 1 | A | 832 | LEU | CA-CB-CG | 5.35 | 127.60 | 115.30 |
| 1 | A | 796 | MET | CB-CG-SD | 5.33 | 128.40 | 112.40 |
| 1 | A | 1726 | LEU | CA-CB-CG | 5.33 | 127.56 | 115.30 |
| 1 | A | 1301 | MET | CA-CB-CG | 5.30 | 122.32 | 113.30 |
| 1 | A | 1335 | ARG | CA-CB-CG | 5.29 | 125.04 | 113.40 |
| 1 | A | 2049 | LEU | CA-CB-CG | 5.26 | 127.41 | 115.30 |
| 1 | A | 1105 | LYS | CA-CB-CG | 5.26 | 124.97 | 113.40 |
| 1 | A | 453 | GLU | CA-CB-CG | 5.26 | 124.96 | 113.40 |
| 1 | A | 712 | LEU | CA-CB-CG | 5.15 | 127.15 | 115.30 |
| 1 | A | 680 | LEU | CA-CB-CG | 5.08 | 126.99 | 115.30 |
| 1 | A | 729 | LEU | CA-CB-CG | 5.08 | 126.99 | 115.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 1014 | VAL | Peptide |

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 12717 | 0 | 12818 | 198 | 0 |
| All | All | 12717 | 0 | 12818 | 198 | 0 |

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 8.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1108:SER:HA | 1:A:1219:LYS:O | 1.75 | 0.86 |
| 1:A:1099:SER:O | 1:A:1103:SER:HB3 | 1.94 | 0.68 |
| 1:A:1549:VAL:O | 1:A:1555:ARG:HA | 1.96 | 0.66 |
| 1:A:799:GLN:HA | 1:A:802:ILE:HD12 | 1.78 | 0.65 |
| 1:A:692:THR:O | 1:A:696:ASN:HB2 | 1.98 | 0.64 |
| 1:A:1872:ARG:HA | 1:A:1875:ARG:HB2 | 1.81 | 0.63 |
| 1:A:718:THR:OG1 | 1:A:1603:GLU:OE1 | 2.17 | 0.62 |
| 1:A:1328:ILE:HA | 1:A:1333:LYS:HD2 | 1.80 | 0.62 |
| 1:A:1659:GLU:OE2 | 1:A:1957:LYS:NZ | 2.33 | 0.62 |
| 1:A:1596:LEU:HD13 | 1:A:1658:ILE:HG23 | 1.82 | 0.61 |
| 1:A:1351:ILE:HG13 | 1:A:1352:LEU:HD12 | 1.83 | 0.61 |
| 1:A:586:CYS:SG | 1:A:587:MET:N | 2.74 | 0.60 |
| 1:A:1899:LYS:O | 1:A:1903:MET:CB | 2.49 | 0.60 |
| 1:A:341:ARG:HD2 | 1:A:1045:PRO:HG2 | 1.83 | 0.60 |
| 1:A:718:THR:HA | 1:A:721:LYS:HD2 | 1.82 | 0.60 |
| 1:A:1677:VAL:HG21 | 1:A:1726:LEU:HD21 | 1.83 | 0.60 |
| 1:A:1086:GLU:HA | 1:A:1091:PHE:HB2 | 1.84 | 0.60 |
| 1:A:1099:SER:HA | 1:A:1102:LYS:HG2 | 1.84 | 0.60 |
| 1:A:1350:ASP:O | 1:A:1354:LYS:NZ | 2.34 | 0.59 |
| 1:A:1581:TYR:HB2 | 1:A:1620:TYR:HB3 | 1.84 | 0.59 |
| 1:A:851:LYS:HE2 | 1:A:1602:ASN:HB2 | 1.83 | 0.59 |
| 1:A:491:ASN:O | 1:A:495:ASN:ND2 | 2.36 | 0.58 |
| 1:A:897:LEU:HA | 1:A:900:MET:HG2 | 1.85 | 0.58 |
| 1:A:678:PHE:HB2 | 1:A:882:ILE:HG23 | 1.84 | 0.57 |
| 1:A:1218:LEU:HD13 | 1:A:1282:SER:HB3 | 1.85 | 0.57 |
| 1:A:1157:GLU:OE1 | 1:A:1212:ARG:NH2 | 2.37 | 0.57 |
| 1:A:494:ILE:HD12 | 1:A:498:ARG:HH22 | 1.69 | 0.56 |
| 1:A:1545:SER:OG | 1:A:1546:SER:N | 2.39 | 0.55 |
| 1:A:1727:ILE:HD13 | 1:A:1914:PHE:HB2 | 1.89 | 0.54 |
| 1:A:1098:ILE:HG22 | 1:A:1100:THR:H | 1.71 | 0.54 |
| 1:A:854:ASN:HA | 1:A:857:GLU:HG2 | 1.88 | 0.54 |
| 1:A:1690:VAL:HG12 | 1:A:1922:ILE:HD11 | 1.88 | 0.54 |
| 1:A:1049:MET:N | 1:A:1049:MET:SD | 2.81 | 0.54 |
| 1:A:1899:LYS:O | 1:A:1903:MET:HB2 | 2.08 | 0.53 |
| 1:A:1899:LYS:O | 1:A:1903:MET:HB3 | 2.08 | 0.53 |
| 1:A:1955:THR:OG1 | 1:A:1956:GLU:N | 2.41 | 0.53 |
| 1:A:588:LYS:O | 1:A:595:LYS:NZ | 2.42 | 0.53 |
| 1:A:1641:LEU:HD23 | 1:A:1646:ILE:HD13 | 1.91 | 0.53 |
| 1:A:1649:ASN:HD21 | 1:A:1729:LEU:HD11 | 1.73 | 0.53 |
| 1:A:1249:GLY:HA2 | 1:A:1255:LYS:H | 1.73 | 0.53 |
| 1:A:471:SER:OG | 1:A:472:MET:N | 2.43 | 0.52 |
| 1:A:924:ILE:HA | 1:A:928:PHE:HB2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:993:GLU:HG2 | 1:A:1562:ILE:HD12 | 1.92 | 0.52 |
| 1:A:747:VAL:O | 1:A:750:ARG:NH1 | 2.42 | 0.52 |
| 1:A:880:ILE:HA | 1:A:883:ASN:HD22 | 1.75 | 0.52 |
| 1:A:534:LEU:O | 1:A:538:SER:OG | 2.27 | 0.52 |
| 1:A:875:MET:SD | 1:A:875:MET:N | 2.69 | 0.52 |
| 1:A:1209:LEU:HD21 | 1:A:1445:ASN:HB2 | 1.92 | 0.52 |
| 1:A:1505:GLU:HG3 | 1:A:1508:LYS:HB2 | 1.91 | 0.52 |
| 1:A:587:MET:SD | 1:A:590:THR:OG1 | 2.64 | 0.52 |
| 1:A:873:MET:HB2 | 1:A:878:LYS:HG3 | 1.91 | 0.52 |
| 1:A:702:PRO:HG2 | 1:A:716:LEU:HD12 | 1.92 | 0.51 |
| 1:A:742:SER:OG | 1:A:832:LEU:O | 2.27 | 0.51 |
| 1:A:2036:VAL:O | 1:A:2040:ASN:HB2 | 2.09 | 0.51 |
| 1:A:1961:VAL:HG13 | 1:A:1962:VAL:HG23 | 1.92 | 0.51 |
| 1:A:730:ALA:HB1 | 1:A:733:HIS:HB2 | 1.92 | 0.51 |
| 1:A:1278:ASP:OD1 | 1:A:1278:ASP:N | 2.42 | 0.51 |
| 1:A:1432:GLU:HB3 | 1:A:1436:GLY:HA3 | 1.93 | 0.51 |
| 1:A:1962:VAL:HG21 | 1:A:1975:TYR:HE2 | 1.75 | 0.51 |
| 1:A:1484:ASP:N | 1:A:1484:ASP:OD1 | 2.44 | 0.50 |
| 1:A:1492:HIS:HB3 | 1:A:1495:ASP:HB2 | 1.93 | 0.50 |
| 1:A:1670:ASP:N | 1:A:1670:ASP:OD1 | 2.43 | 0.50 |
| 1:A:1384:ILE:HG21 | 1:A:1398:MET:HE2 | 1.93 | 0.50 |
| 1:A:702:PRO:O | 1:A:705:LEU:HB2 | 2.11 | 0.50 |
| 1:A:323:SER:OG | 1:A:324:LYS:N | 2.45 | 0.50 |
| 1:A:1726:LEU:HA | 1:A:1729:LEU:HB3 | 1.94 | 0.50 |
| 1:A:1319:GLN:HG3 | 1:A:1327:SER:HB2 | 1.93 | 0.50 |
| 1:A:1120:GLU:O | 1:A:1124:ASN:ND2 | 2.44 | 0.50 |
| 1:A:1082:ARG:NH2 | 1:A:1394:GLU:OE2 | 2.45 | 0.50 |
| 1:A:1764:GLU:HA | 1:A:1767:LEU:HG | 1.93 | 0.50 |
| 1:A:1209:LEU:HG | 1:A:1215:VAL:HG21 | 1.94 | 0.49 |
| 1:A:507:VAL:HA | 1:A:812:PHE:HB3 | 1.95 | 0.49 |
| 1:A:798:ASP:N | 1:A:798:ASP:OD1 | 2.44 | 0.49 |
| 1:A:534:LEU:HD21 | 1:A:789:LEU:HD11 | 1.93 | 0.49 |
| 1:A:1470:MET:HE2 | 1:A:1489:TRP:HB3 | 1.95 | 0.49 |
| 1:A:1657:PRO:HB2 | 1:A:1660:PRO:HD2 | 1.93 | 0.49 |
| 1:A:437:ILE:HB | 1:A:921:LYS:HD2 | 1.94 | 0.49 |
| 1:A:879:GLN:O | 1:A:883:ASN:ND2 | 2.46 | 0.49 |
| 1:A:1932:PRO:O | 1:A:1936:SER:HB3 | 2.13 | 0.49 |
| 1:A:1520:GLU:OE2 | 1:A:1524:ARG:NH1 | 2.46 | 0.49 |
| 1:A:1687:LEU:HD12 | 1:A:1690:VAL:HB | 1.95 | 0.49 |
| 1:A:981:LYS:N | 1:A:985:THR:O | 2.43 | 0.48 |
| 1:A:1075:ILE:HD11 | 1:A:1317:VAL:HG13 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1363:PHE:CE1 | 1:A:1549:VAL:HA | 2.48 | 0.48 |
| 1:A:1538:ASN:O | 1:A:1542:SER:OG | 2.22 | 0.48 |
| 1:A:827:LEU:HD12 | 1:A:832:LEU:HD23 | 1.95 | 0.48 |
| 1:A:1090:ASP:HB3 | 1:A:1093:SER:HB2 | 1.94 | 0.48 |
| 1:A:2040:ASN:HA | 1:A:2043:ILE:HG12 | 1.96 | 0.48 |
| 1:A:919:ASN:HB2 | 1:A:923:TYR:HB2 | 1.96 | 0.47 |
| 1:A:1372:SER:OG | 1:A:1452:ASN:OD1 | 2.28 | 0.47 |
| 1:A:806:LYS:O | 1:A:823:ARG:NH1 | 2.35 | 0.47 |
| 1:A:1896:MET:O | 1:A:1900:ILE:HD12 | 2.14 | 0.47 |
| 1:A:2014:LEU:HD23 | 1:A:2025:ALA:HB2 | 1.96 | 0.47 |
| 1:A:1311:GLU:OE1 | 1:A:1459:ASN:N | 2.40 | 0.47 |
| 1:A:586:CYS:HA | 1:A:756:SER:HA | 1.95 | 0.47 |
| 1:A:1329:SER:OG | 1:A:1332:ASN:OD1 | 2.32 | 0.47 |
| 1:A:1109:GLN:HG3 | 1:A:1221:LYS:HD3 | 1.96 | 0.47 |
| 1:A:1834:LEU:HD21 | 1:A:1996:ASN:HB2 | 1.97 | 0.47 |
| 1:A:1238:MET:SD | 1:A:1238:MET:N | 2.80 | 0.47 |
| 1:A:1480:TYR:HE1 | 1:A:1483:CYS:HB2 | 1.80 | 0.47 |
| 1:A:1541:LYS:HA | 1:A:1541:LYS:HD2 | 1.73 | 0.47 |
| 1:A:2019:ASP:N | 1:A:2019:ASP:OD1 | 2.47 | 0.47 |
| 1:A:803:CYS:HB3 | 1:A:804:TYR:HD2 | 1.80 | 0.46 |
| 1:A:1129:ASP:HB3 | 1:A:1132:ASN:HB2 | 1.95 | 0.46 |
| 1:A:1912:CYS:HB2 | 1:A:2034:ARG:HG3 | 1.98 | 0.46 |
| 1:A:829:GLN:HA | 1:A:832:LEU:HG | 1.98 | 0.46 |
| 1:A:1335:ARG:HH12 | 1:A:1552:ILE:HD11 | 1.80 | 0.46 |
| 1:A:1943:ARG:NH2 | 1:A:1969:VAL:O | 2.42 | 0.46 |
| 1:A:476:PRO:HG2 | 1:A:790:HIS:HB3 | 1.96 | 0.46 |
| 1:A:1222:LYS:O | 1:A:1224:SER:N | 2.46 | 0.46 |
| 1:A:821:ILE:HD13 | 1:A:821:ILE:HA | 1.85 | 0.46 |
| 1:A:1732:LYS:HD3 | 1:A:1903:MET:HG2 | 1.98 | 0.46 |
| 1:A:1565:TYR:CE1 | 1:A:1601:PRO:HD3 | 2.50 | 0.45 |
| 1:A:2062:PRO:HB3 | 1:A:2066:LYS:HD3 | 1.98 | 0.45 |
| 1:A:490:ASN:OD1 | 1:A:761:THR:OG1 | 2.33 | 0.45 |
| 1:A:1440:LYS:O | 1:A:1443:THR:OG1 | 2.19 | 0.45 |
| 1:A:674:LYS:NZ | 1:A:883:ASN:OD1 | 2.41 | 0.45 |
| 1:A:1589:SER:HA | 1:A:1592:VAL:HB | 1.99 | 0.45 |
| 1:A:785:PRO:HG3 | 1:A:826:ARG:HE | 1.82 | 0.45 |
| 1:A:852:LYS:HD2 | 1:A:994:ASP:HB3 | 1.97 | 0.45 |
| 1:A:426:ARG:HH12 | 1:A:1532:SER:HB2 | 1.82 | 0.45 |
| 1:A:395:LYS:HE2 | 1:A:404:HIS:HB2 | 1.97 | 0.45 |
| 1:A:1154:ARG:HH21 | 1:A:1209:LEU:HA | 1.81 | 0.45 |
| 1:A:1231:VAL:HG13 | 1:A:1235:HIS:CE1 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:878:LYS:O | 1:A:882:ILE:HG13 | 2.17 | 0.44 |
| 1:A:398:LEU:O | 1:A:402:LYS:NZ | 2.43 | 0.44 |
| 1:A:1209:LEU:HD23 | 1:A:1215:VAL:HG11 | 1.98 | 0.44 |
| 1:A:1663:ILE:HG22 | 1:A:1664:LEU:HD23 | 2.00 | 0.44 |
| 1:A:1753:THR:HG23 | 1:A:1755:ILE:H | 1.81 | 0.44 |
| 1:A:1024:PRO:HB3 | 1:A:1452:ASN:HD22 | 1.82 | 0.44 |
| 1:A:1784:LYS:NZ | 1:A:1819:MET:SD | 2.74 | 0.44 |
| 1:A:842:VAL:HG12 | 1:A:892:GLY:HA3 | 1.99 | 0.44 |
| 1:A:852:LYS:HA | 1:A:852:LYS:HD3 | 1.72 | 0.44 |
| 1:A:1145:ILE:HD11 | 1:A:1177:ILE:HD12 | 1.99 | 0.44 |
| 1:A:2038:ALA:HA | 1:A:2041:TYR:CE2 | 2.53 | 0.44 |
| 1:A:1973:ALA:HA | 1:A:2085:TYR:HA | 2.00 | 0.44 |
| 1:A:869:ASN:N | 1:A:869:ASN:OD1 | 2.48 | 0.43 |
| 1:A:1308:TYR:O | 1:A:1312:HIS:HB2 | 2.19 | 0.43 |
| 1:A:594:ASN:O | 1:A:598:TYR:HB2 | 2.19 | 0.43 |
| 1:A:1372:SER:OG | 1:A:1453:TRP:O | 2.36 | 0.43 |
| 1:A:1531:LYS:HD3 | 1:A:1531:LYS:HA | 1.75 | 0.43 |
| 1:A:1282:SER:O | 1:A:1298:LEU:HB2 | 2.19 | 0.43 |
| 1:A:1315:LYS:HE3 | 1:A:1315:LYS:HB2 | 1.74 | 0.43 |
| 1:A:696:ASN:HB3 | 1:A:700:LYS:HE2 | 2.01 | 0.43 |
| 1:A:1217:VAL:HG11 | 1:A:1415:THR:HG22 | 2.01 | 0.43 |
| 1:A:1014:VAL:HG12 | 1:A:1017:LEU:HD23 | 1.99 | 0.43 |
| 1:A:1554:GLU:H | 1:A:1564:LEU:HD13 | 1.83 | 0.43 |
| 1:A:1602:ASN:HA | 1:A:1953:PHE:CE2 | 2.54 | 0.43 |
| 1:A:1371:TRP:HZ3 | 1:A:1535:ILE:HG23 | 1.84 | 0.43 |
| 1:A:1410:LYS:HE3 | 1:A:1448:PRO:HG3 | 2.00 | 0.43 |
| 1:A:1622:MET:HB2 | 1:A:1628:ASN:HB3 | 2.00 | 0.43 |
| 1:A:1901:LEU:HD23 | 1:A:1901:LEU:HA | 1.86 | 0.43 |
| 1:A:1339:THR:HG21 | 1:A:2084:ILE:HB | 1.99 | 0.43 |
| 1:A:2053:ASN:OD1 | 1:A:2053:ASN:N | 2.51 | 0.43 |
| 1:A:1112:ILE:HB | 1:A:1216:THR:HG23 | 2.01 | 0.43 |
| 1:A:1370:LYS:HD3 | 1:A:1370:LYS:HA | 1.63 | 0.43 |
| 1:A:472:MET:N | 1:A:472:MET:SD | 2.92 | 0.43 |
| 1:A:1414:PRO:HD2 | 1:A:1417:ILE:HD11 | 2.01 | 0.43 |
| 1:A:2047:ASN:HB3 | 1:A:2066:LYS:HD2 | 2.01 | 0.42 |
| 1:A:1687:LEU:O | 1:A:1691:LYS:HD2 | 2.19 | 0.42 |
| 1:A:2023:THR:HB | 1:A:2060:SER:HB3 | 2.02 | 0.42 |
| 1:A:993:GLU:O | 1:A:997:ASN:ND2 | 2.52 | 0.42 |
| 1:A:1278:ASP:HB2 | 1:A:1302:LYS:HG3 | 2.01 | 0.42 |
| 1:A:1425:GLN:HG3 | 1:A:1432:GLU:HG2 | 2.01 | 0.42 |
| 1:A:741:PHE:CE1 | 1:A:769:LEU:HD21 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1373:ALA:HA | 1:A:1452:ASN:HA | 2.01 | 0.42 |
| 1:A:1671:GLN:NE2 | 1:A:1924:ASP:OD2 | 2.53 | 0.42 |
| 1:A:437:ILE:HG21 | 1:A:443:ALA:HB2 | 2.01 | 0.42 |
| 1:A:1357:LYS:HE2 | 1:A:1357:LYS:HB2 | 1.87 | 0.42 |
| 1:A:373:ASP:HA | 1:A:376:ILE:HG12 | 2.02 | 0.41 |
| 1:A:2076:ASN:N | 1:A:2076:ASN:OD1 | 2.53 | 0.41 |
| 1:A:1109:GLN:NE2 | 1:A:1226:GLU:OE2 | 2.53 | 0.41 |
| 1:A:760:LEU:HB2 | 1:A:769:LEU:HB2 | 2.01 | 0.41 |
| 1:A:470:PHE:HD1 | 1:A:470:PHE:HA | 1.77 | 0.41 |
| 1:A:1410:LYS:HB3 | 1:A:1446:THR:HG22 | 2.01 | 0.41 |
| 1:A:2084:ILE:HD12 | 1:A:2084:ILE:HA | 1.88 | 0.41 |
| 1:A:498:ARG:HH21 | 1:A:538:SER:HB2 | 1.86 | 0.41 |
| 1:A:1380:TYR:O | 1:A:1384:ILE:HD12 | 2.21 | 0.41 |
| 1:A:707:ILE:HD13 | 1:A:707:ILE:HA | 1.92 | 0.41 |
| 1:A:1122:LEU:HD23 | 1:A:1169:LEU:HD13 | 2.02 | 0.41 |
| 1:A:1133:TRP:HH2 | 1:A:1176:ILE:HD12 | 1.85 | 0.41 |
| 1:A:1345:ILE:HD11 | 1:A:1488:ARG:HB2 | 2.03 | 0.41 |
| 1:A:1507:ASP:O | 1:A:1511:THR:HG23 | 2.21 | 0.41 |
| 1:A:1642:LYS:HD3 | 1:A:1642:LYS:HA | 1.83 | 0.41 |
| 1:A:737:ASP:O | 1:A:741:PHE:HB2 | 2.20 | 0.41 |
| 1:A:788:ALA:HB1 | 1:A:790:HIS:NE2 | 2.36 | 0.41 |
| 1:A:831:ARG:HH11 | 1:A:895:THR:HG22 | 1.86 | 0.41 |
| 1:A:1769:LYS:HD3 | 1:A:1769:LYS:HA | 1.78 | 0.41 |
| 1:A:355:GLU:OE1 | 1:A:404:HIS:NE2 | 2.47 | 0.40 |
| 1:A:1605:ILE:H | 1:A:1605:ILE:HD12 | 1.86 | 0.40 |
| 1:A:1262:MET:O | 1:A:1266:VAL:HG23 | 2.22 | 0.40 |
| 1:A:479:GLU:OE2 | 1:A:479:GLU:N | 2.54 | 0.40 |
| 1:A:924:ILE:HD12 | 1:A:924:ILE:H | 1.86 | 0.40 |
| 1:A:1281:VAL:HG11 | 1:A:1454:LEU:HD12 | 2.03 | 0.40 |
| 1:A:1940:CYS:HB2 | 1:A:1945:ARG:HB3 | 2.02 | 0.40 |
| 1:A:1043:ILE:HD12 | 1:A:1043:ILE:HA | 1.98 | 0.40 |
| 1:A:1337:LEU:HD23 | 1:A:1337:LEU:HA | 1.98 | 0.40 |
| 1:A:1944:LYS:HD3 | 1:A:1959:ILE:HD12 | 2.03 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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 | 1556/1776 (88%) | 1433 (92%) | 118 (8%) | 5 (0%) | 37 71 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1755 | ILE |
| 1 | A | 1045 | PRO |
| 1 | A | 1044 | TYR |
| 1 | A | 1106 | LYS |
| 1 | A | 1853 | SER |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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 | 1453/1646 (88%) | 1396 (96%) | 57 (4%) | 27 50 |

All (57) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 321 | TRP |
| 1 | A | 324 | LYS |
| 1 | A | 378 | ASP |
| 1 | A | 409 | GLN |
| 1 | A | 414 | SER |
| 1 | A | 415 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 433 | LYS |
| 1 | A | 451 | TYR |
| 1 | A | 470 | PHE |
| 1 | A | 742 | SER |
| 1 | A | 799 | GLN |
| 1 | A | 809 | TYR |
| 1 | A | 875 | MET |
| 1 | A | 906 | MET |
| 1 | A | 911 | PHE |
| 1 | A | 937 | ASP |
| 1 | A | 995 | LEU |
| 1 | A | 996 | TYR |
| 1 | A | 1005 | MET |
| 1 | A | 1037 | PHE |
| 1 | A | 1049 | MET |
| 1 | A | 1054 | ASP |
| 1 | A | 1202 | GLU |
| 1 | A | 1246 | MET |
| 1 | A | 1262 | MET |
| 1 | A | 1314 | PHE |
| 1 | A | 1316 | HIS |
| 1 | A | 1340 | LEU |
| 1 | A | 1348 | TYR |
| 1 | A | 1354 | LYS |
| 1 | A | 1363 | PHE |
| 1 | A | 1415 | THR |
| 1 | A | 1463 | SER |
| 1 | A | 1480 | TYR |
| 1 | A | 1509 | MET |
| 1 | A | 1521 | MET |
| 1 | A | 1545 | SER |
| 1 | A | 1548 | GLU |
| 1 | A | 1564 | LEU |
| 1 | A | 1566 | CYS |
| 1 | A | 1620 | TYR |
| 1 | A | 1648 | THR |
| 1 | A | 1661 | LEU |
| 1 | A | 1704 | PHE |
| 1 | A | 1844 | LEU |
| 1 | A | 1898 | LYS |
| 1 | A | 1917 | CYS |
| 1 | A | 1979 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2008 | MET |
| 1 | A | 2026 | PHE |
| 1 | A | 2037 | LYS |
| 1 | A | 2042 | MET |
| 1 | A | 2047 | ASN |
| 1 | A | 2056 | PHE |
| 1 | A | 2061 | PHE |
| 1 | A | 2067 | PHE |
| 1 | A | 2071 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 495 | ASN |
| 1 | A | 1124 | ASN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

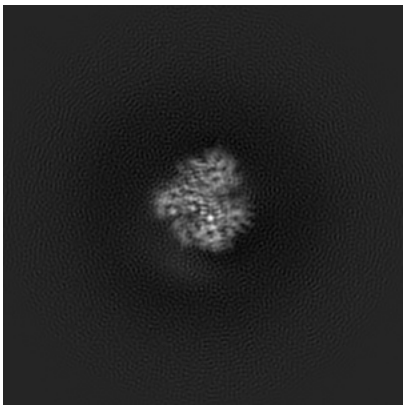
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37256. These allow visual inspection of the internal detail of the map and identification of artifacts.

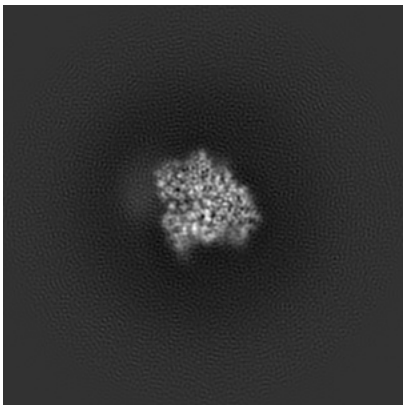
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

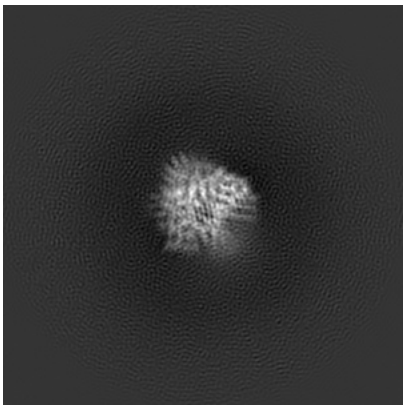
### 6.1.1 Primary map



X

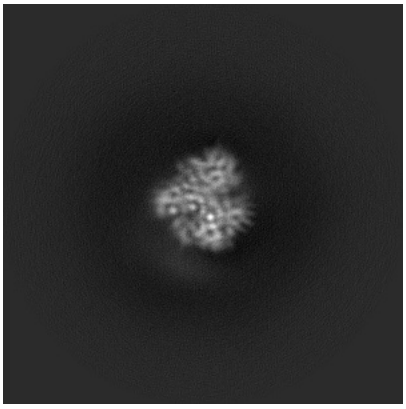


Y

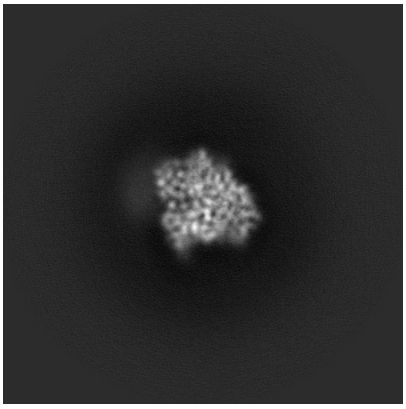


Z

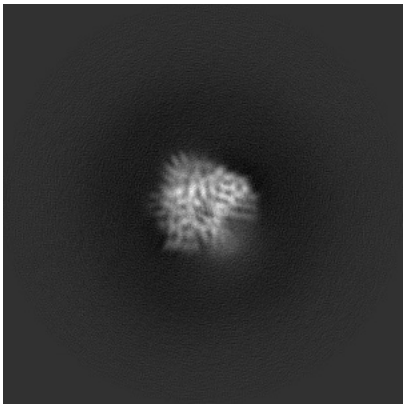
### 6.1.2 Raw map



X



Y

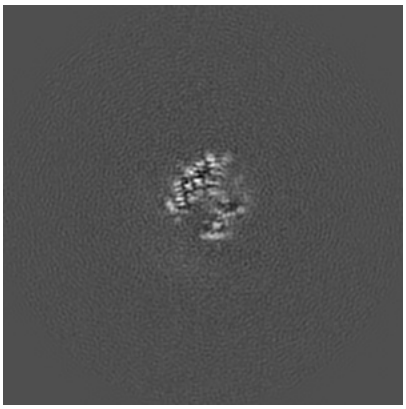


Z

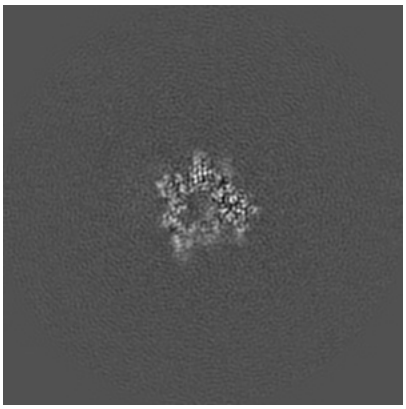
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

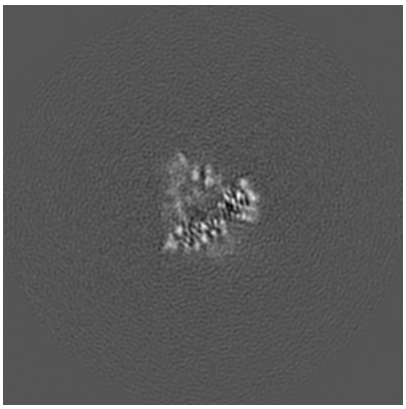
### 6.2.1 Primary map



X Index: 180

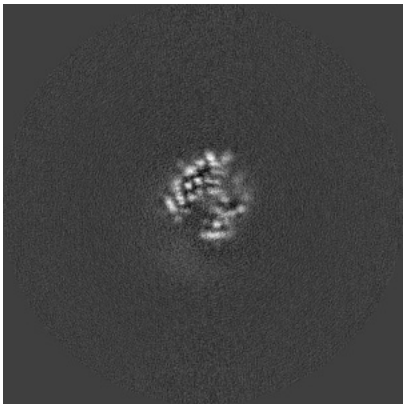


Y Index: 180

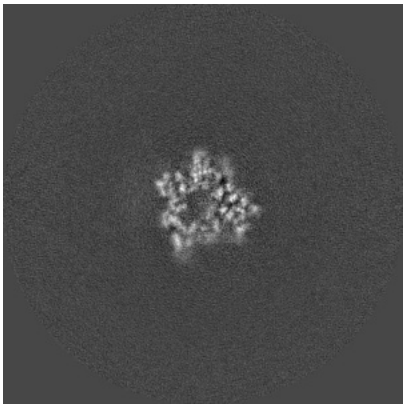


Z Index: 180

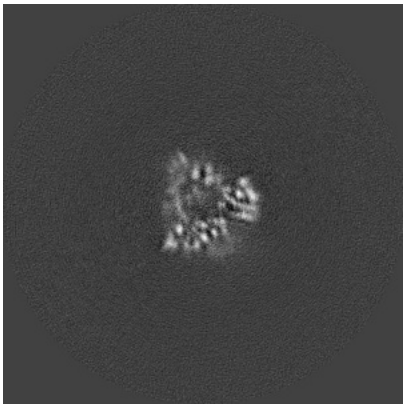
### 6.2.2 Raw map



X Index: 180



Y Index: 180

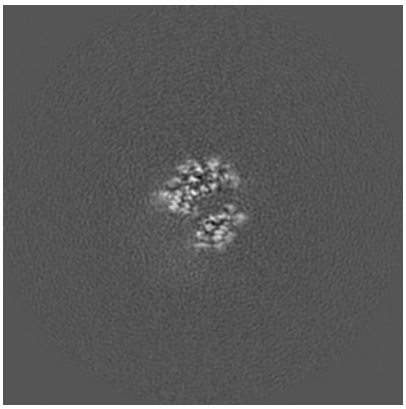


Z Index: 180

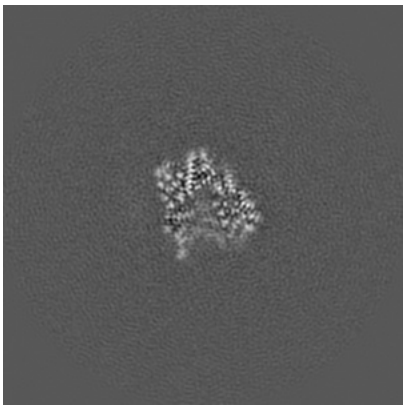
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

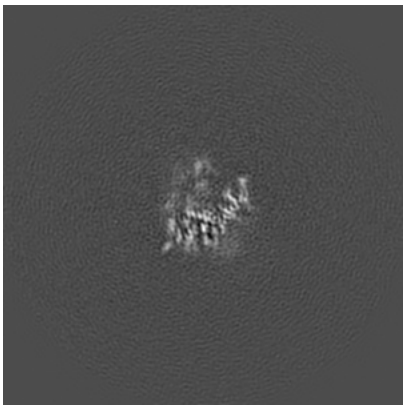
### 6.3.1 Primary map



X Index: 190

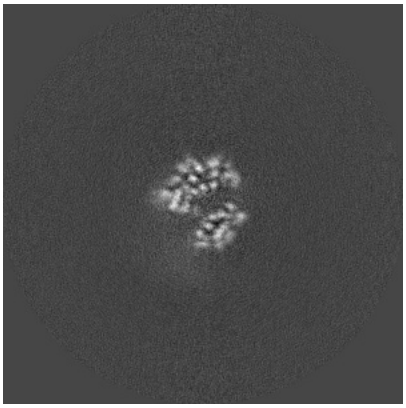


Y Index: 187

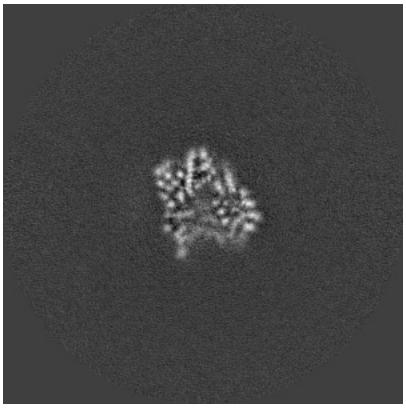


Z Index: 185

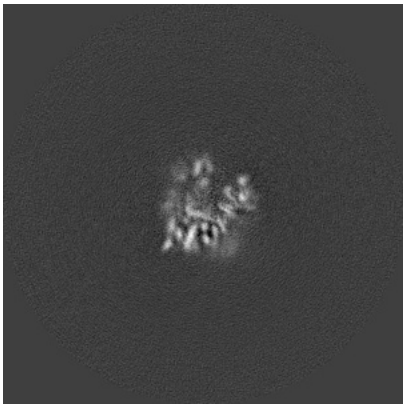
### 6.3.2 Raw map



X Index: 190



Y Index: 187

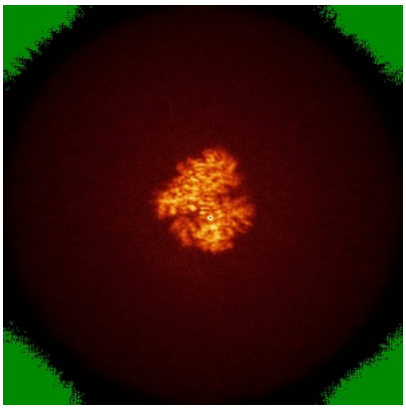


Z Index: 184

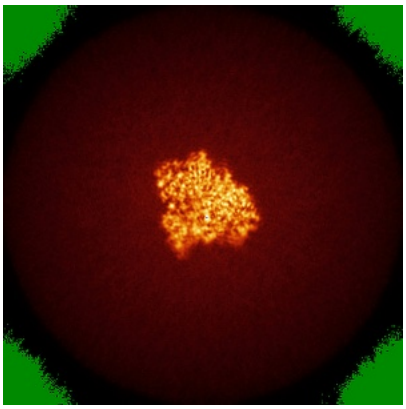
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

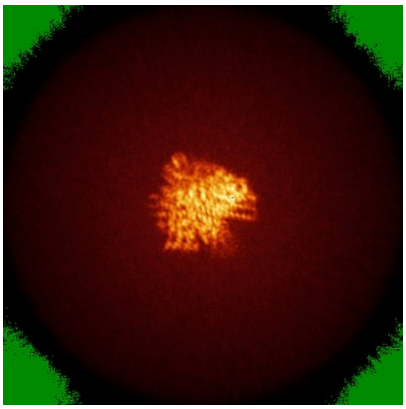
### 6.4.1 Primary map



X

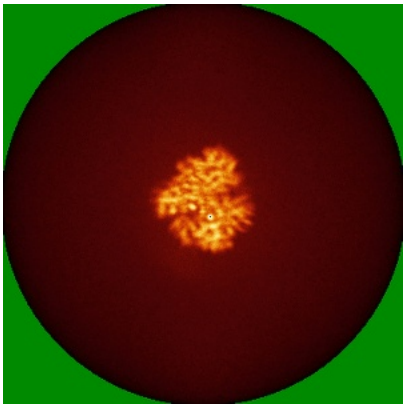


Y

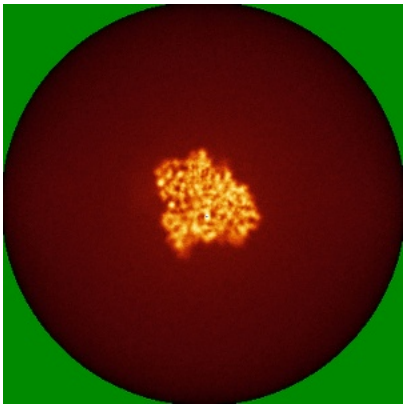


Z

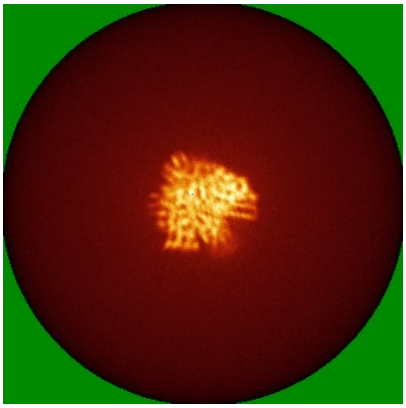
### 6.4.2 Raw map



X



Y

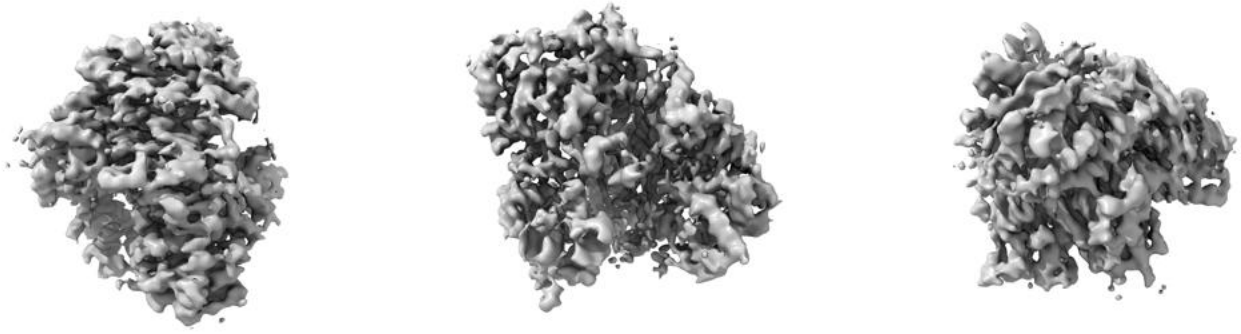


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

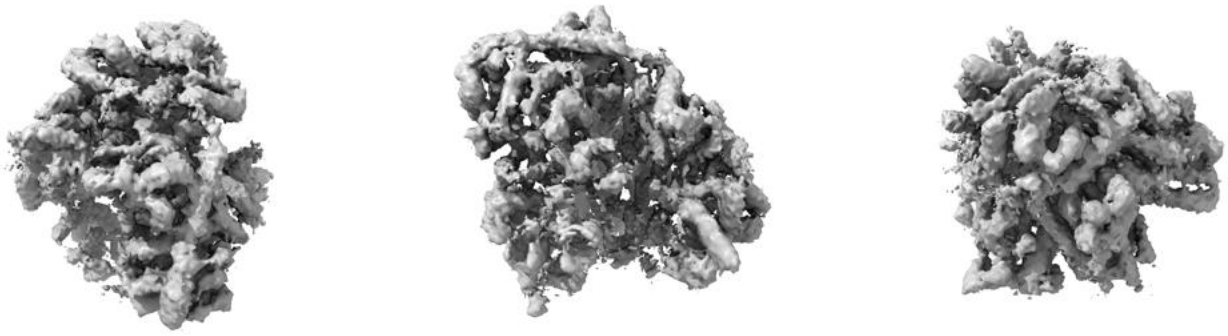
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

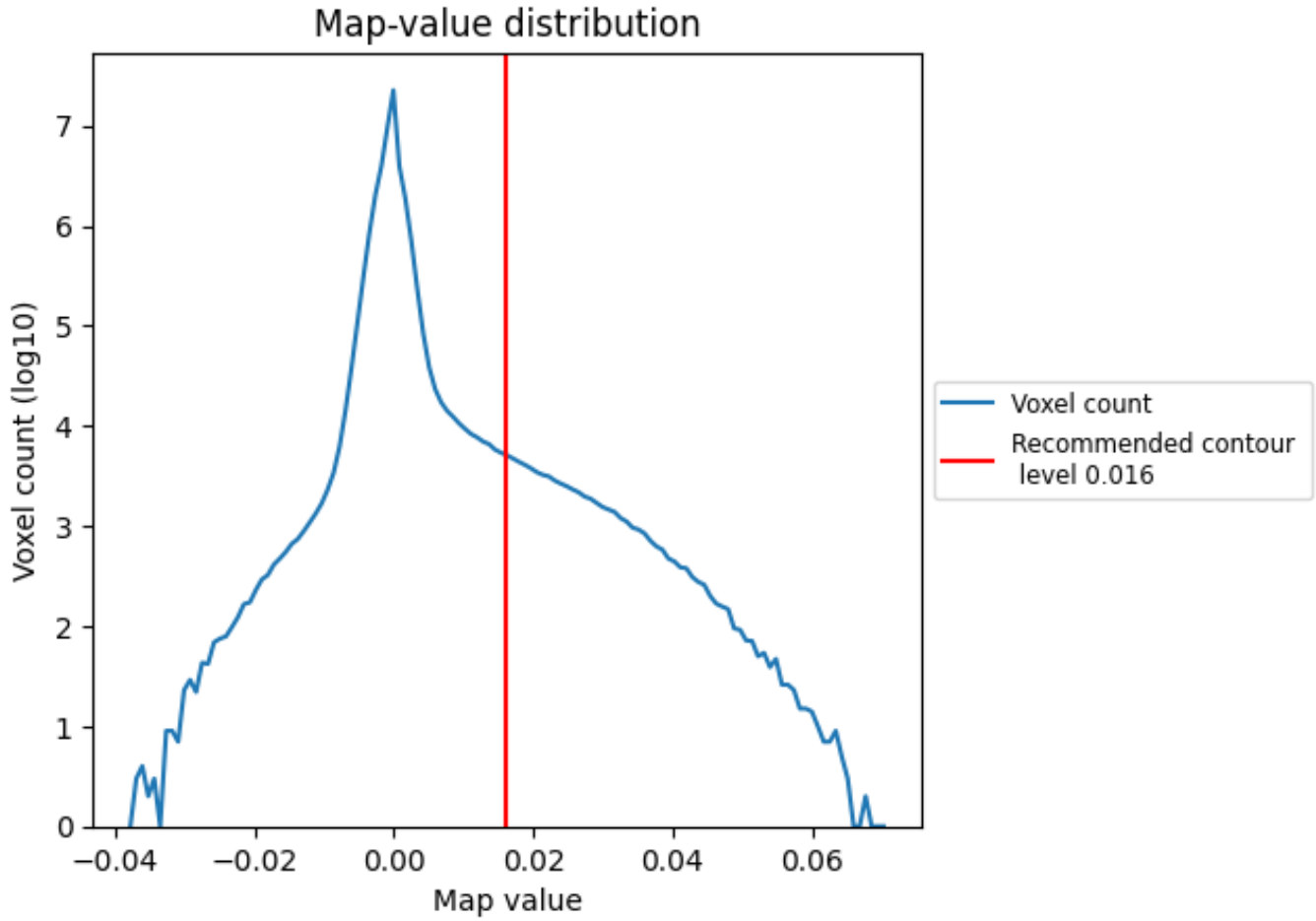
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

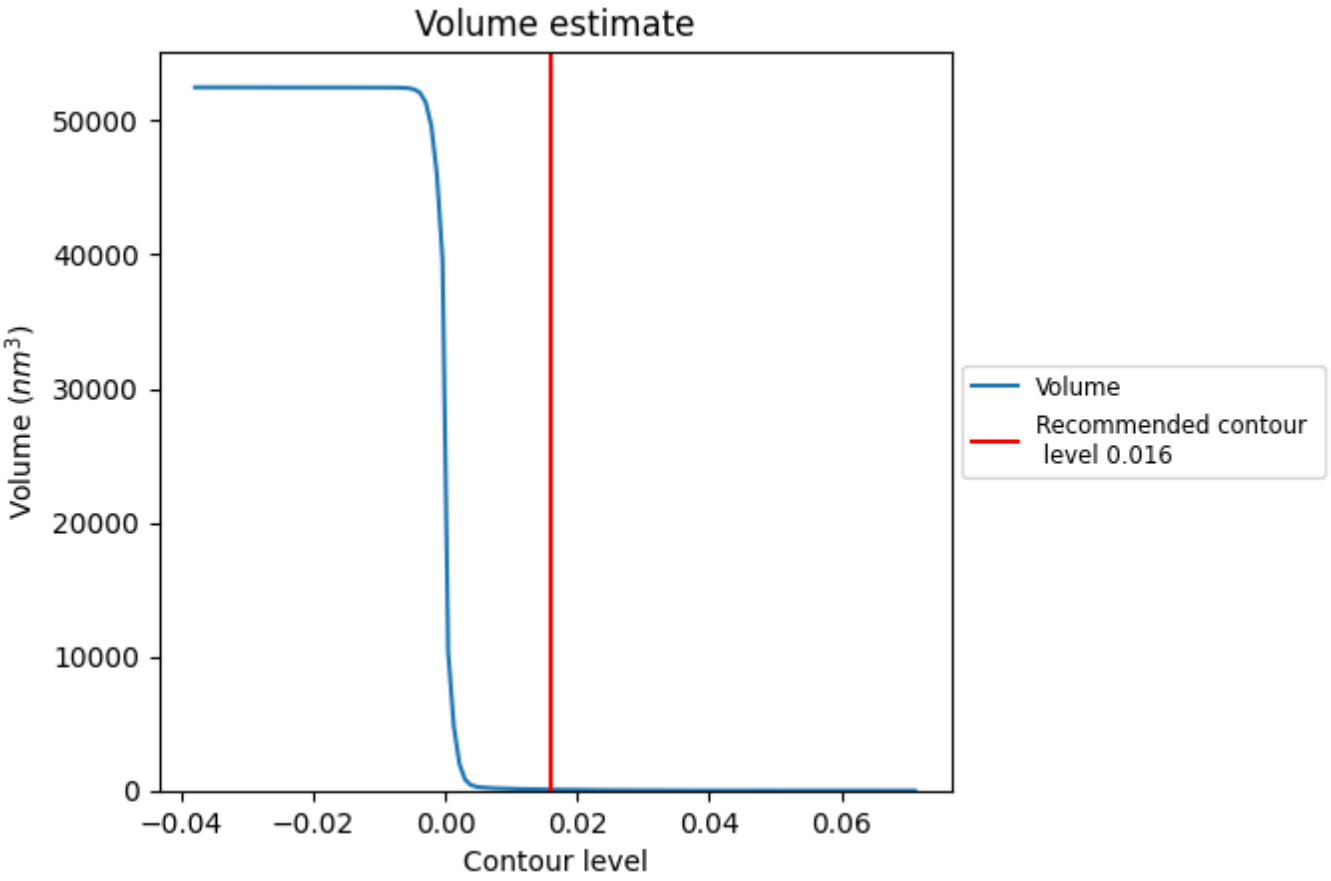
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

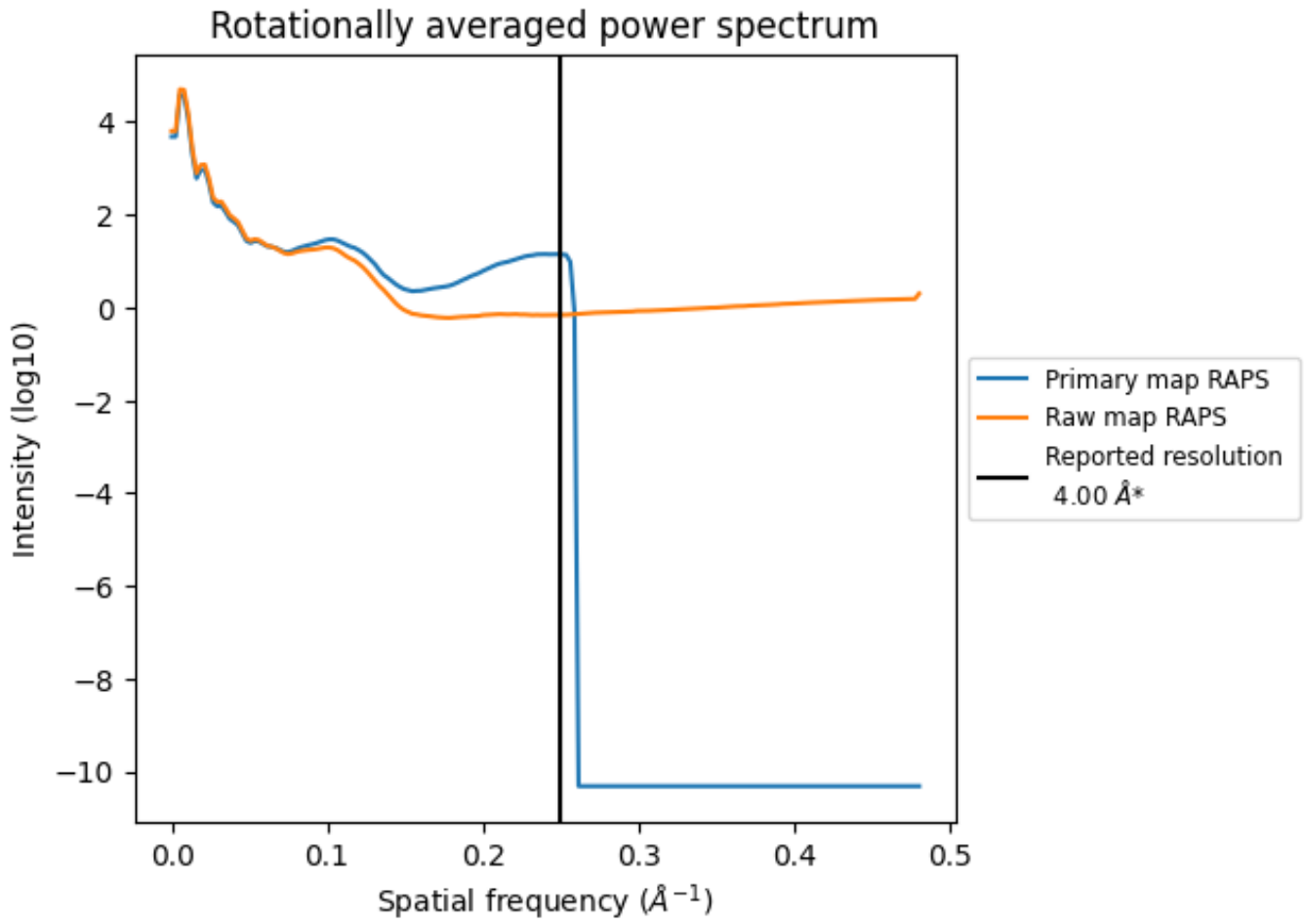
## 7.2 Volume estimate




The volume at the recommended contour level is 75 $nm^3$; this corresponds to an approximate mass of 68 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

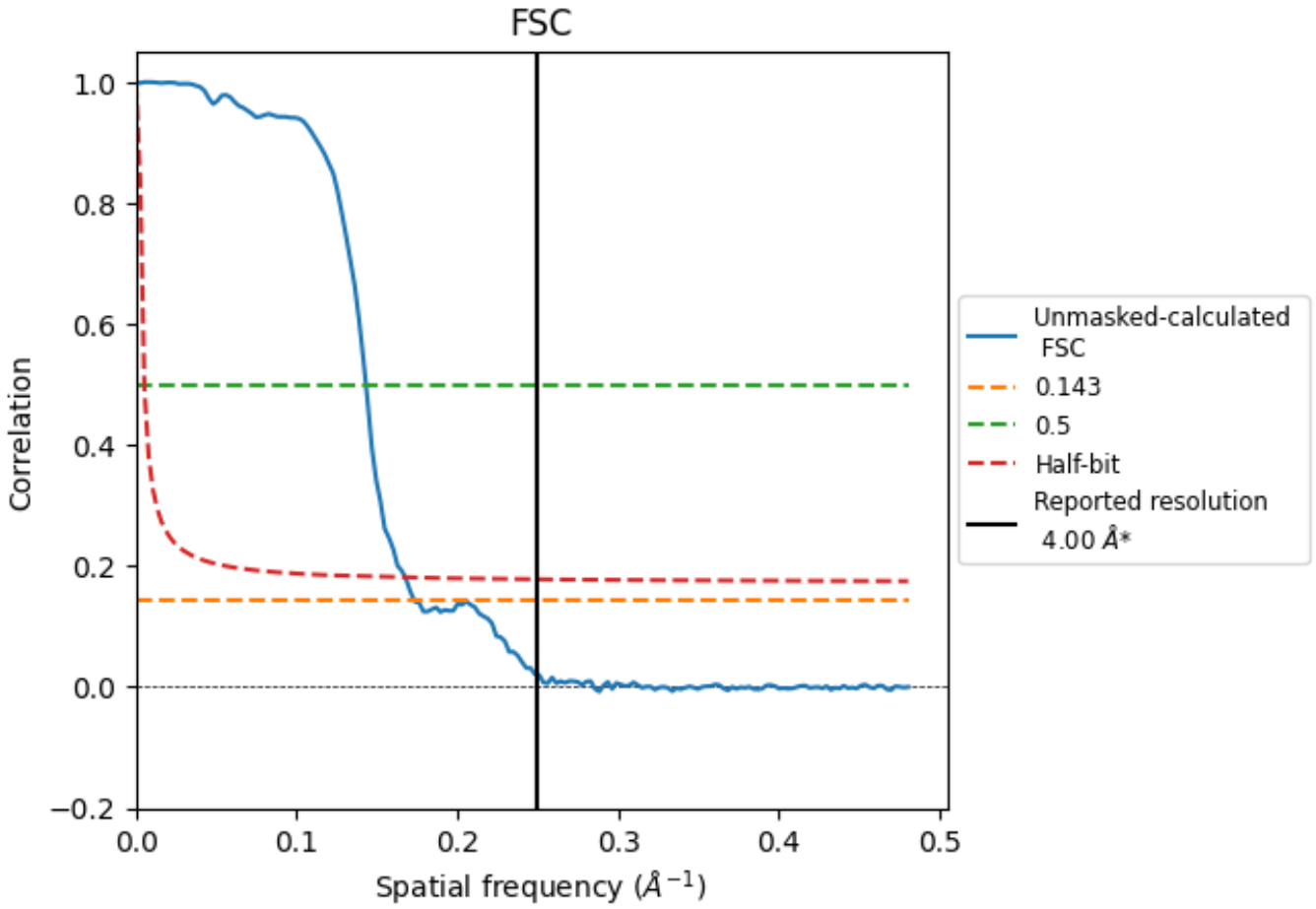



*Reported resolution corresponds to spatial frequency of 0.250 Å$^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.250 Å$^{-1}$

## 8.2 Resolution estimates (i)

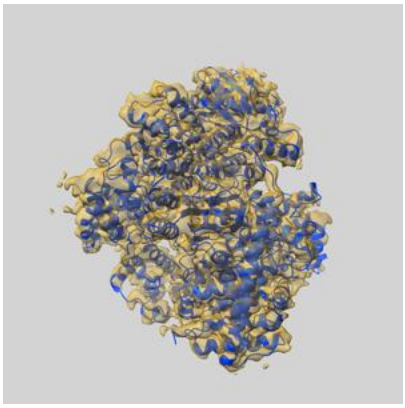
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.00 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 5.77 | 6.98 | 5.97 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.77 differs from the reported value 4.0 by more than 10 %

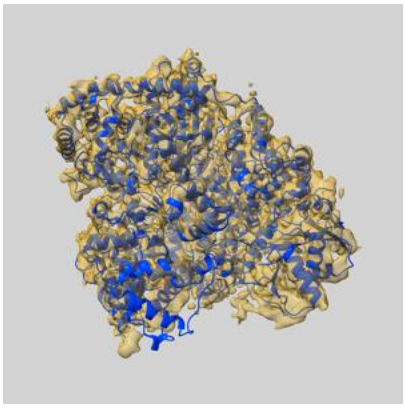
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37256 and PDB model 8KIA. Per-residue inclusion information can be found in section 3 on page 4.

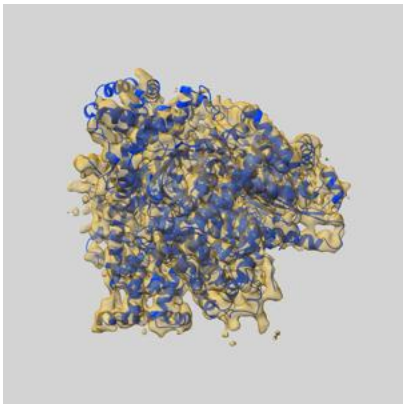
## 9.1 Map-model overlay



X



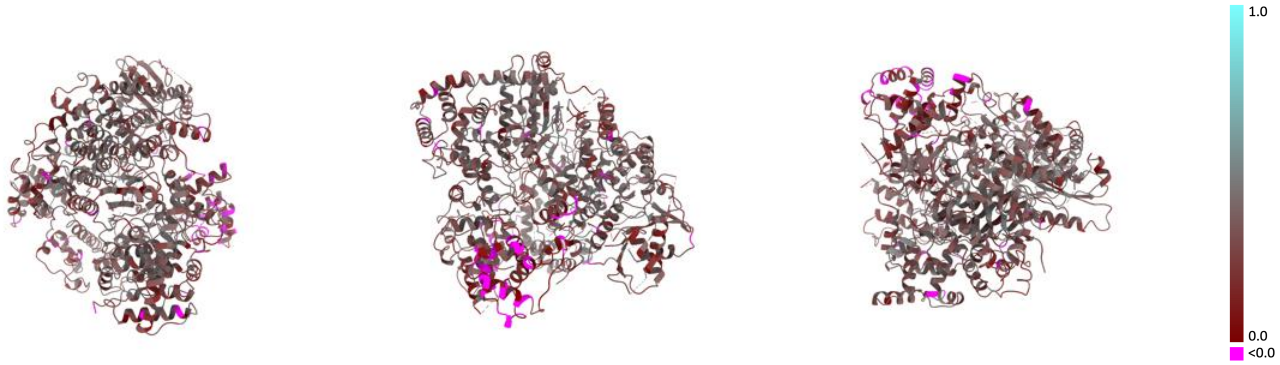
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

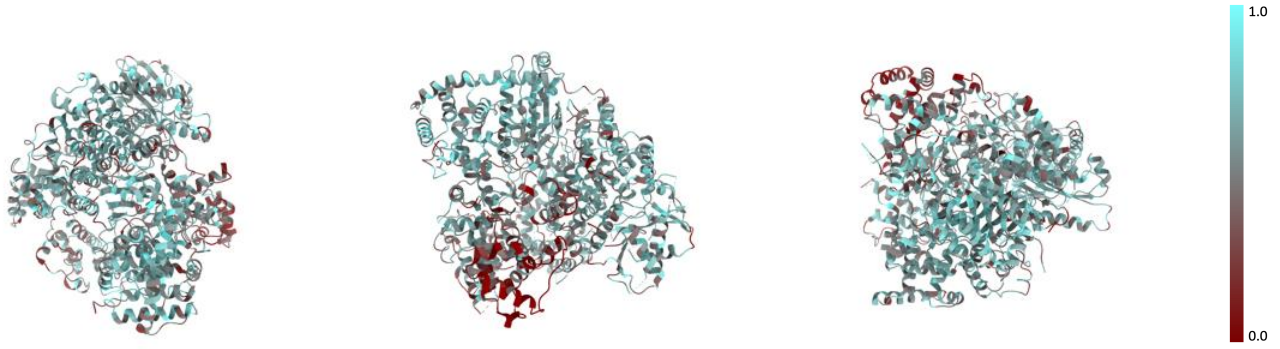
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

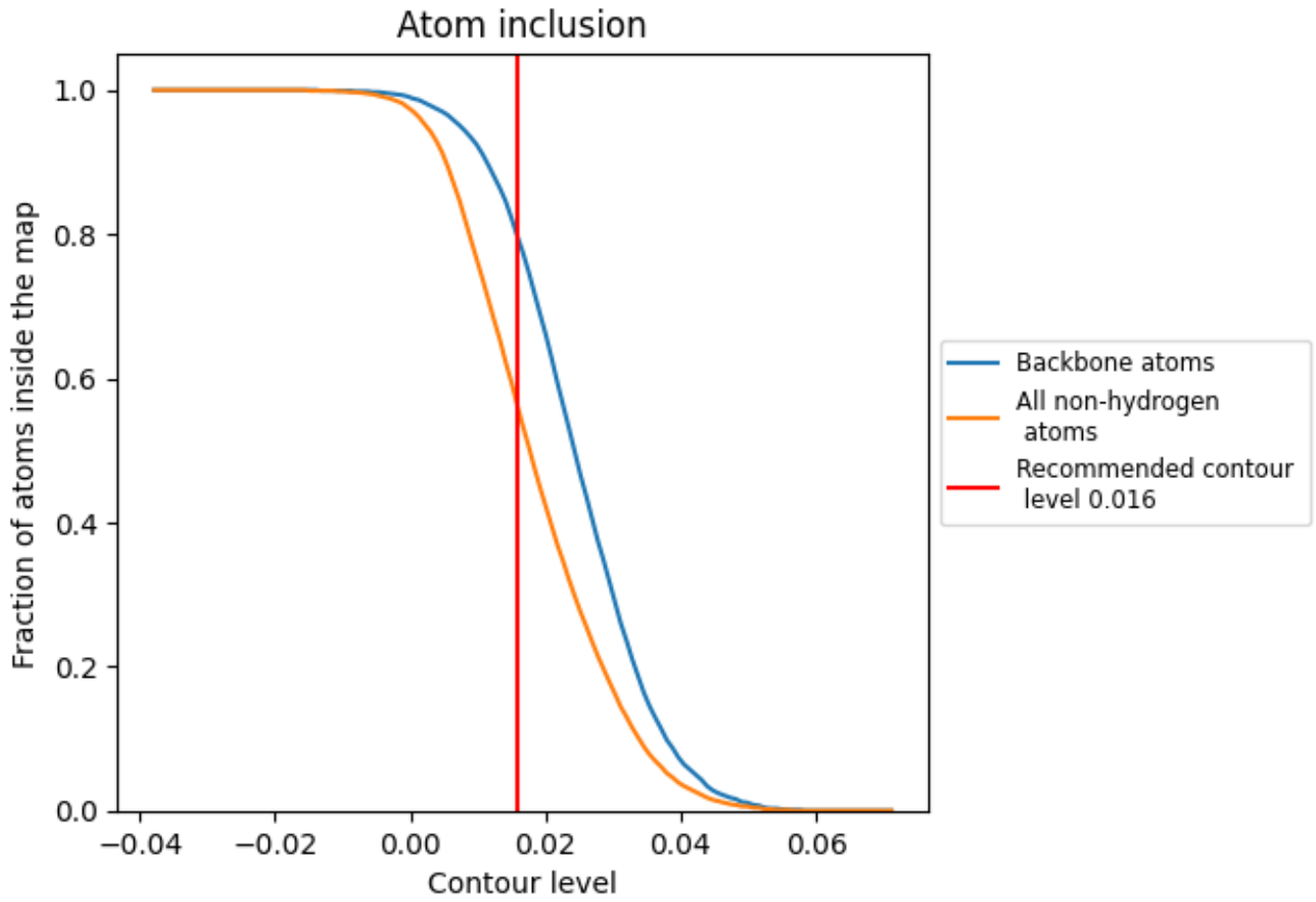
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

## 9.4 Atom inclusion (i)




At the recommended contour level, 79% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5570 | 0.3030 |
| A | 0.5570 | 0.3030 |