Full wwPDB EM Validation Report ⓘ

Oct 28, 2023 – 12:22 PM EDT

PDB ID	:	8TX1
EMDB ID	:	EMD-41674
Title	:	Characterization of the Chlamydomonas Flagellar Mastigoneme Filament Structure at 3.6A
Authors	:	Yue, W.; Kai, Z.
Deposited on	:	2023-08-22
Resolution	:	3.62 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:

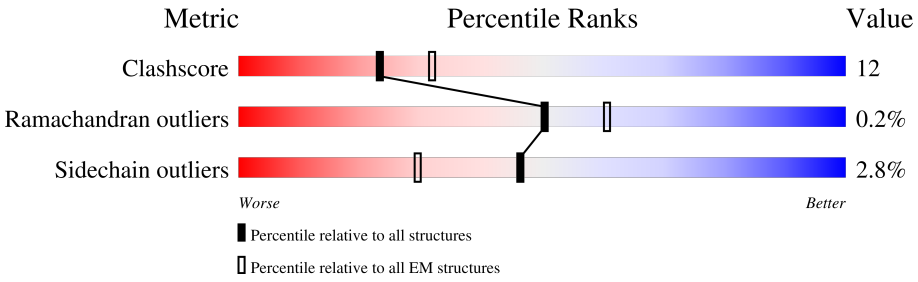
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.62 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1987	11% 68% 26% • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13687 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 Mastigoneme-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1894	13687	8643	2234	2727	83	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	VAL	conflict	UNP Q8LRM7
A	142	LEU	THR	conflict	UNP Q8LRM7
A	143	ALA	GLY	conflict	UNP Q8LRM7
A	144	SER	LEU	conflict	UNP Q8LRM7
A	145	LYS	GLU	conflict	UNP Q8LRM7
A	146	THR	ASP	conflict	UNP Q8LRM7
A	147	VAL	GLY	conflict	UNP Q8LRM7
A	149	ILE	HIS	conflict	UNP Q8LRM7
A	150	TYR	LEU	conflict	UNP Q8LRM7
A	151	VAL	CYS	conflict	UNP Q8LRM7
A	517	ARG	LYS	conflict	UNP Q8LRM7
A	530	GLU	GLY	conflict	UNP Q8LRM7
A	619	THR	ALA	conflict	UNP Q8LRM7
A	800	SER	THR	conflict	UNP Q8LRM7
A	820	SER	PHE	conflict	UNP Q8LRM7
A	?	-	GLY	deletion	UNP Q8LRM7
A	?	-	THR	deletion	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	GLY	deletion	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	TYR	deletion	UNP Q8LRM7
A	?	-	PHE	deletion	UNP Q8LRM7
A	?	-	LEU	deletion	UNP Q8LRM7
A	1399	LYS	ARG	conflict	UNP Q8LRM7
A	?	-	PRO	deletion	UNP Q8LRM7
A	?	-	GLU	deletion	UNP Q8LRM7
A	1868	PRO	ALA	conflict	UNP Q8LRM7
A	1897	PRO	GLN	conflict	UNP Q8LRM7

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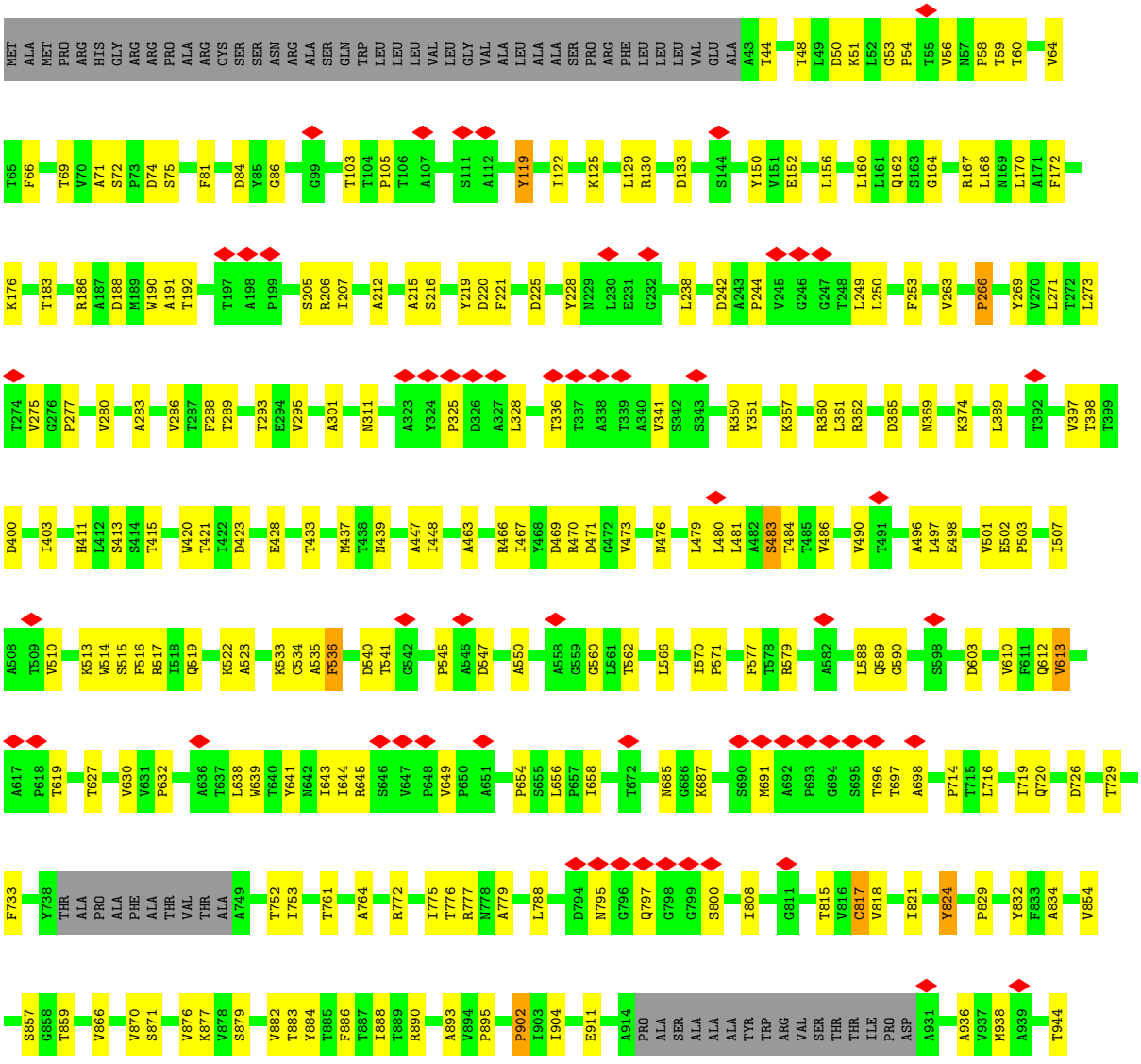
Chain	Residue	Modelled	Actual	Comment	Reference
A	1914	PRO	ARG	conflict	UNP Q8LRM7
A	1915	PRO	ARG	conflict	UNP Q8LRM7
A	1917	PRO	HIS	conflict	UNP Q8LRM7
A	1919	SER	ALA	conflict	UNP Q8LRM7
A	1920	PRO	ARG	conflict	UNP Q8LRM7
A	1921	PRO	ARG	conflict	UNP Q8LRM7
A	1924	ASN	THR	conflict	UNP Q8LRM7
A	1925	ARG	ALA	conflict	UNP Q8LRM7
A	1926	SER	LEU	conflict	UNP Q8LRM7
A	1935	SER	PRO	conflict	UNP Q8LRM7
A	1978	ASP	-	expression tag	UNP Q8LRM7
A	1979	ALA	-	expression tag	UNP Q8LRM7
A	1980	GLU	-	expression tag	UNP Q8LRM7
A	1981	MET	-	expression tag	UNP Q8LRM7
A	1982	GLN	-	expression tag	UNP Q8LRM7
A	1983	PRO	-	expression tag	UNP Q8LRM7
A	1984	GLN	-	expression tag	UNP Q8LRM7
A	1985	ASP	-	expression tag	UNP Q8LRM7
A	1986	ASP	-	expression tag	UNP Q8LRM7
A	1987	GLU	-	expression tag	UNP Q8LRM7

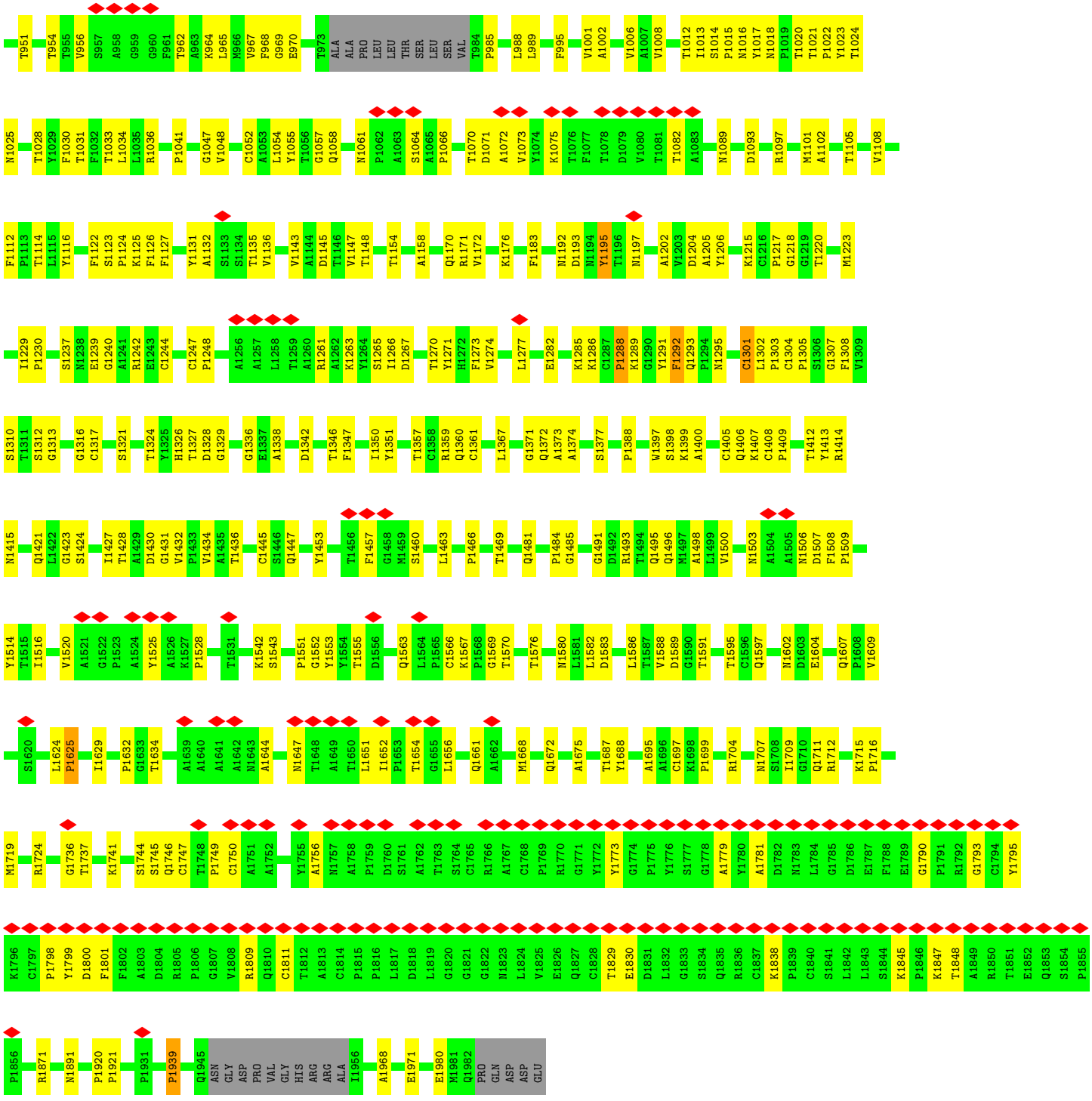
3 Residue-property plots (i)

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: Mastigoneme-like protein

Chain A:




T951 T954 T955 V956 S957 A958 G959 G960 F961 T962 A963 K964 L965 M966 V967 F968 G969 E970 T973 ALA ALA PRO LEU LEU THR SER LEU SER VAL T984 P985 L988 L989 F995 V1001 A1002 V1006 A1007 V1008 T1012 I1013 S1014 P1015 N1016 Y1017 N1018 P1019 T1020 T1021 P1022 Y1023 T1024
N1025 T1028 Y1029 F1030 T1031 F1032 T1033 L1034 L1035 R1036 P1041 G1047 V1048 C1052 A1053 L1054 Y1055 T1056 G1057 Q1058 N1061 P1062 A1063 S1064 A1065 P1066 T1070 D1071 A1072 V1073 Y1074 K1075 T1076 F1077 T1078 D1079 V1080 T1081 T1082 A1083 N1089 D1093 R1097 M1101 A1102 T1105 V1108
F1112 P1113 T1114 L1115 Y1116 F1122 S1123 P1124 K1125 F1126 F1127 Y1131 A1132 S1133 S1134 T1135 V1136 V1143 A1144 D1145 T1146 V1147 T1148 T1154 A1158 Q1170 R1171 V1172 K1176 F1183 N1192 D1193 N1194 Y1195 T1196 N1197 A1202 V1203 D1204 A1205 Y1206 K1215 C1216 P1217 G1218 G1219 T1220 M1223
I1229 P1230 S1237 N1238 E1239 G1240 A1241 R1242 E1243 C1244 C1247 P1248 A1256 A1257 L1258 T1259 A1260 R1261 A1262 K1263 Y1264 S1265 I1266 D1267 T1270 Y1271 H1272 F1273 V1274 L1277 E1282 K1285 K1286 C1287 P1288 K1289 G1290 Y1291 F1292 Q1293 P1294 N1295 C1301 L1302 P1303 C1304 P1305 S1306 G1307 F1308 V1309
S1310 T1311 S1312 G1313 G1316 C1317 S1321 T1324 Y1325 H1326 T1327 D1328 G1329 G1336 E1337 A1338 D1342 T1346 F1347 I1350 Y1351 T1357 C1358 R1359 Q1360 C1361 L1367 G1371 Q1372 A1373 A1374 S1377 P1388 W1397 S1398 K1399 A1400 C1405 Q1406 K1407 C1408 P1409 T1412 Y1413 R1414
N1415 Q1421 L1422 G1423 S1424 I1427 T1428 A1429 D1430 G1431 V1432 P1433 V1434 A1435 T1436 C1445 S1446 Q1447 Y1453 T1456 F1457 G1458 M1459 S1460 L1463 P1466 T1469 Q1481 P1484 G1485 G1491 D1492 R1493 T1494 Q1495 Q1496 M1497 A1498 L1499 V1500 N1503 A1504 A1505 N1506 D1507 F1508 P1509
Y1514 T1515 I1516 V1520 A1521 G1522 P1523 A1524 Y1525 A1526 K1527 P1528 T1531 K1542 S1543 P1551 G1552 Y1553 Y1554 T1555 D1556 Q1563 L1564 P1565 C1566 K1567 P1568 G1569 T1570 T1576 N1580 L1581 L1582 D1583 L1586 T1587 V1588 D1589 G1590 T1591 T1595 C1596 Q1597 N1602 D1603 E1604 Q1607 P1608 V1609
S1620 L1624 P1625 I1629 P1632 G1633 T1634 A1639 A1640 A1641 A1642 N1643 A1644 N1647 T1648 A1649 T1650 L1651 I1652 P1653 T1654 G1655 L1656 Q1661 A1662 M1668 Q1672 A1675 T1687 Y1688 A1695 A1696 C1697 K1698 P1699 R1704 N1707 S1708 I1709 G1710 Q1711 R1712 K1715 P1716
M1719 R1724 G1736 T1737 K1741 S1744 S1745 Q1746 C1747 T1748 P1749 C1750 A1751 A1752 Y1755 A1756 N1757 A1758 P1759 D1760 S1761 A1762 T1763 S1764 C1765 R1766 A1767 C1768 P1769 R1770 G1771 Y1772 Y1773 G1774 P1775 Y1776 S1777 G1778 A1779 Y1780 A1781 D1782 N1783 L1784 G1785 D1786 E1787 F1788 E1789 G1790 P1791 R1792 G1793 C1794 Y1795
K1796 C1797 P1798 Y1799 D1800 F1801 F1802 A1803 D1804 R1805 P1806 G1807 V1808 R1809 Q1810 C1811 T1812 A1813 C1814 P1815 P1816 L1817 D1818 L1819 G1820 G1821 G1822 N1823 L1824 V1825 E1826 Q1827 C1828 T1829 E1830 D1831 L1832 G1833 S1834 Q1835 R1836 C1837 K1838 P1839 C1840 S1841 L1842 L1843 S1844 K1845 P1846 K1847 T1848 A1849 R1850 T1851 E1852 Q1853 S1854 P1855
P1856 R1871 N1891 P1920 P1921 P1931 P1939 Q1945 ASN GLY ASP PRO VAL GLY HIS ARG ARG ALA I1956 A1968 E1971 E1980 M1981 Q1982 PRO GLN ASP ASP GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98875	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.145	Depositor
Minimum map value	-1.930	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.321	Depositor
Map size (Å)	494.7598, 494.7598, 494.7598	wwPDB
Map dimensions	372, 372, 372	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3299994, 1.3299994, 1.3299994	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	0.30	2/14067 (0.0%)	0.59	12/19393 (0.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	902	PRO	CB-CG	-10.08	0.99	1.50
1	A	902	PRO	CG-CD	-6.84	1.28	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	902	PRO	N-CD-CG	-19.37	74.15	103.20
1	A	902	PRO	CA-CB-CG	-17.07	71.58	104.00
1	A	902	PRO	CB-CG-CD	13.28	158.28	106.50
1	A	902	PRO	CA-N-CD	-12.86	93.50	111.50
1	A	1267	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	266	PRO	CA-N-CD	-6.27	102.72	111.50
1	A	1528	PRO	CA-N-CD	-5.94	103.18	111.50
1	A	1625	PRO	CA-N-CD	-5.78	103.41	111.50
1	A	1939	PRO	N-CA-CB	5.50	109.90	103.30
1	A	105	PRO	CA-N-CD	-5.37	103.98	111.50
1	A	1288	PRO	CA-N-CD	-5.18	104.25	111.50
1	A	1625	PRO	N-CD-CG	-5.05	95.62	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1282	GLU	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	13687	0	13237	332	0
All	All	13687	0	13237	332	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 12.

All (332) 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:1055:TYR:O	1:A:1124:PRO:HA	1.40	1.17
1:A:238:LEU:HB3	1:A:253:PHE:HB3	1.61	0.82
1:A:1223:MET:SD	1:A:1242:ARG:NH1	2.53	0.80
1:A:1336:GLY:H	1:A:1357:THR:HG22	1.45	0.80
1:A:1220:THR:HG22	1:A:1230:PRO:HB3	1.62	0.80
1:A:1289:LYS:HG2	1:A:1312:SER:H	1.44	0.78
1:A:167:ARG:HD2	1:A:170:LEU:HB3	1.67	0.76
1:A:1057:GLY:HA3	1:A:1123:SER:H	1.48	0.76
1:A:761:THR:HB	1:A:857:SER:HB3	1.69	0.74
1:A:535:ALA:HB2	1:A:560:GLY:HA2	1.70	0.73
1:A:1466:PRO:O	1:A:1542:LYS:NZ	2.17	0.73
1:A:968:PHE:HA	1:A:988:LEU:HD23	1.69	0.73
1:A:1493:ARG:HH22	1:A:1551:PRO:HD3	1.52	0.73
1:A:1397:TRP:CD1	1:A:1408:CYS:HB3	2.25	0.72
1:A:967:VAL:HB	1:A:989:LEU:HG	1.74	0.69
1:A:1055:TYR:HB3	1:A:1125:LYS:HG2	1.73	0.69
1:A:644:ILE:HG22	1:A:697:THR:HG22	1.74	0.69
1:A:890:ARG:HG2	1:A:893:ALA:H	1.56	0.68
1:A:1192:ASN:HD21	1:A:1204:ASP:HA	1.59	0.68
1:A:1506:ASN:HD21	1:A:1508:PHE:HB3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLN:HG2	1:A:610:VAL:HG13	1.74	0.68
1:A:1801:PHE:HB3	1:A:1811:CYS:HB3	1.74	0.68
1:A:658:ILE:HA	1:A:720:GLN:HB2	1.75	0.66
1:A:397:VAL:HG12	1:A:398:THR:HG23	1.78	0.66
1:A:1583:ASP:OD1	1:A:1597:GLN:NE2	2.29	0.66
1:A:1192:ASN:ND2	1:A:1206:TYR:O	2.26	0.66
1:A:176:LYS:HD2	1:A:220:ASP:HB3	1.78	0.66
1:A:753:ILE:HG13	1:A:775:ILE:HG12	1.77	0.65
1:A:890:ARG:HH22	1:A:895:PRO:HG2	1.62	0.65
1:A:411:HIS:ND1	1:A:413:SER:O	2.30	0.65
1:A:84:ASP:OD2	1:A:130:ARG:NH2	2.29	0.65
1:A:360:ARG:HD2	1:A:362:ARG:HD2	1.79	0.65
1:A:439:ASN:HD21	1:A:447:ALA:H	1.46	0.64
1:A:1066:PRO:HB3	1:A:1073:VAL:HG11	1.78	0.63
1:A:51:LYS:HG2	1:A:53:GLY:H	1.62	0.63
1:A:1672:GLN:N	1:A:1672:GLN:OE1	2.32	0.62
1:A:829:PRO:HA	1:A:854:VAL:O	1.99	0.62
1:A:1604:GLU:OE1	1:A:1604:GLU:N	2.32	0.62
1:A:1018:ASN:OD1	1:A:1020:THR:OG1	2.14	0.62
1:A:1302:LEU:HD12	1:A:1303:PRO:HD2	1.82	0.62
1:A:1328:ASP:O	1:A:1359:ARG:NH2	2.33	0.62
1:A:627:THR:O	1:A:638:LEU:HB3	2.00	0.61
1:A:1520:VAL:HG21	1:A:1525:TYR:HA	1.81	0.61
1:A:522:LYS:NZ	1:A:523:ALA:O	2.32	0.61
1:A:1195:TYR:O	1:A:1215:LYS:NZ	2.31	0.61
1:A:685:ASN:O	1:A:687:LYS:NZ	2.31	0.61
1:A:1013:ILE:O	1:A:1016:ASN:ND2	2.34	0.61
1:A:788:LEU:HD12	1:A:815:THR:HG21	1.83	0.61
1:A:466:ARG:HH12	1:A:481:LEU:H	1.49	0.60
1:A:466:ARG:NH2	1:A:467:ILE:O	2.34	0.60
1:A:1289:LYS:NZ	1:A:1338:ALA:HA	2.17	0.60
1:A:1415:ASN:ND2	1:A:1460:SER:OG	2.34	0.60
1:A:191:ALA:O	1:A:207:ILE:N	2.29	0.60
1:A:1075:LYS:HG2	1:A:1136:VAL:HG21	1.84	0.59
1:A:466:ARG:NH2	1:A:479:LEU:O	2.35	0.59
1:A:423:ASP:O	1:A:463:ALA:HA	2.03	0.59
1:A:716:LEU:H	1:A:733:PHE:HE1	1.51	0.59
1:A:1326:HIS:HB2	1:A:1373:ALA:HB1	1.84	0.59
1:A:1423:GLY:N	1:A:1434:VAL:O	2.25	0.59
1:A:1229:ILE:HG13	1:A:1230:PRO:HD2	1.83	0.59
1:A:1197:ASN:O	1:A:1215:LYS:NZ	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:THR:OG1	1:A:400:ASP:OD1	2.20	0.58
1:A:271:LEU:HD13	1:A:374:LYS:HD3	1.85	0.58
1:A:1779:ALA:HB1	1:A:1793:GLY:HA2	1.85	0.58
1:A:533:LYS:HB2	1:A:562:THR:HG23	1.85	0.58
1:A:962:THR:OG1	1:A:964:LYS:NZ	2.37	0.58
1:A:1006:VAL:HG22	1:A:1036:ARG:HA	1.85	0.57
1:A:1707:ASN:OD1	1:A:1715:LYS:NZ	2.33	0.57
1:A:1553:TYR:HE1	1:A:1563:GLN:HG2	1.70	0.57
1:A:1498:ALA:HB1	1:A:1500:VAL:HG22	1.85	0.57
1:A:882:VAL:HG21	1:A:951:THR:HG22	1.86	0.57
1:A:879:SER:HB2	1:A:1041:PRO:HA	1.85	0.57
1:A:1310:SER:HB3	1:A:1317:CYS:SG	2.44	0.57
1:A:483:SER:OG	1:A:484:THR:N	2.35	0.56
1:A:498:GLU:HB2	1:A:517:ARG:HE	1.70	0.56
1:A:1580:ASN:ND2	1:A:1609:VAL:HG11	2.20	0.56
1:A:1350:ILE:HG13	1:A:1351:TYR:CD1	2.41	0.56
1:A:1052:CYS:HB3	1:A:1112:PHE:HZ	1.71	0.56
1:A:1218:GLY:HA2	1:A:1239:GLU:HA	1.86	0.56
1:A:1023:TYR:HB3	1:A:1158:ALA:HB2	1.87	0.56
1:A:870:VAL:HG12	1:A:884:TYR:CE1	2.41	0.55
1:A:311:ASN:HB3	1:A:360:ARG:HG2	1.88	0.55
1:A:311:ASN:HB3	1:A:360:ARG:CG	2.35	0.55
1:A:514:TRP:HZ2	1:A:588:LEU:HB2	1.70	0.55
1:A:832:TYR:HE1	1:A:834:ALA:HB2	1.71	0.55
1:A:273:LEU:O	1:A:275:VAL:HG23	2.07	0.55
1:A:192:THR:HG23	1:A:206:ARG:HG3	1.88	0.55
1:A:1582:LEU:HD11	1:A:1586:LEU:HD11	1.89	0.55
1:A:1367:LEU:HD21	1:A:1372:GLN:HB3	1.88	0.55
1:A:1412:THR:HG22	1:A:1447:GLN:HA	1.89	0.55
1:A:566:LEU:HB2	1:A:571:PRO:HG3	1.89	0.55
1:A:772:ARG:HG2	1:A:818:VAL:HG22	1.88	0.55
1:A:1360:GLN:OE1	1:A:1360:GLN:N	2.30	0.54
1:A:1668:MET:HB3	1:A:1712:ARG:HH21	1.71	0.54
1:A:1293:GLN:HE21	1:A:1301:CYS:HA	1.72	0.54
1:A:74:ASP:OD1	1:A:74:ASP:N	2.38	0.54
1:A:277:PRO:HG2	1:A:280:VAL:HB	1.89	0.54
1:A:1054:LEU:HA	1:A:1125:LYS:O	2.07	0.54
1:A:1202:ALA:HB1	1:A:1205:ALA:HB2	1.89	0.54
1:A:1484:PRO:O	1:A:1555:THR:OG1	2.22	0.54
1:A:1724:ARG:HH12	1:A:1745:SER:HB2	1.71	0.54
1:A:507:ILE:HB	1:A:510:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:ASP:O	1:A:1346:THR:OG1	2.24	0.54
1:A:1052:CYS:HB3	1:A:1112:PHE:CZ	2.42	0.54
1:A:1024:THR:OG1	1:A:1025:ASN:N	2.41	0.53
1:A:1304:CYS:HB2	1:A:1305:PRO:HD2	1.90	0.53
1:A:1647:ASN:O	1:A:1651:LEU:N	2.42	0.53
1:A:1709:ILE:O	1:A:1711:GLN:NE2	2.41	0.53
1:A:1428:THR:HG23	1:A:1431:GLY:H	1.73	0.53
1:A:1399:LYS:HD2	1:A:1400:ALA:N	2.23	0.53
1:A:1576:THR:HG23	1:A:1588:VAL:HG11	1.90	0.53
1:A:59:THR:HG22	1:A:60:THR:H	1.73	0.53
1:A:886:PHE:CE1	1:A:965:LEU:HD13	2.43	0.53
1:A:1741:LYS:HB3	1:A:1744:SER:HB3	1.91	0.53
1:A:1048:VAL:HG22	1:A:1101:MET:HB2	1.90	0.53
1:A:1192:ASN:HB2	1:A:1206:TYR:HB2	1.91	0.53
1:A:970:GLU:HG2	1:A:985:PRO:HD2	1.91	0.53
1:A:1736:GLY:HA2	1:A:1756:ALA:HB2	1.90	0.53
1:A:1014:SER:OG	1:A:1015:PRO:HD3	2.09	0.52
1:A:1687:THR:HG22	1:A:1699:PRO:HA	1.90	0.52
1:A:1781:ALA:HA	1:A:1790:GLY:HA3	1.90	0.52
1:A:795:ASN:ND2	1:A:797:GLN:O	2.42	0.52
1:A:1102:ALA:O	1:A:1105:THR:OG1	2.25	0.52
1:A:1421:GLN:HE21	1:A:1447:GLN:HB2	1.74	0.52
1:A:1800:ASP:HA	1:A:1829:THR:HB	1.91	0.52
1:A:190:TRP:HB3	1:A:206:ARG:HB3	1.90	0.52
1:A:360:ARG:CD	1:A:362:ARG:HD2	2.40	0.52
1:A:325:PRO:HB2	1:A:328:LEU:HB3	1.90	0.52
1:A:1028:THR:OG1	1:A:1114:THR:O	2.24	0.52
1:A:808:ILE:HD11	1:A:815:THR:HG22	1.92	0.52
1:A:1242:ARG:HG2	1:A:1242:ARG:HH11	1.75	0.52
1:A:1773:TYR:O	1:A:1795:TYR:N	2.43	0.51
1:A:1127:PHE:HZ	1:A:1145:ASP:HA	1.75	0.51
1:A:167:ARG:HD3	1:A:168:LEU:O	2.11	0.51
1:A:273:LEU:HD11	1:A:361:LEU:HD22	1.92	0.51
1:A:1570:THR:HA	1:A:1595:THR:HA	1.92	0.51
1:A:1580:ASN:HB3	1:A:1656:LEU:HD22	1.91	0.51
1:A:1217:PRO:HD2	1:A:1220:THR:OG1	2.10	0.51
1:A:72:SER:OG	1:A:75:SER:O	2.28	0.51
1:A:1289:LYS:HG2	1:A:1312:SER:N	2.22	0.51
1:A:1408:CYS:HB2	1:A:1409:PRO:HD2	1.91	0.51
1:A:501:VAL:HG12	1:A:503:PRO:HD2	1.92	0.50
1:A:1629:ILE:HG21	1:A:1675:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1644:ALA:HB2	1:A:1656:LEU:HB2	1.91	0.50
1:A:172:PHE:N	1:A:225:ASP:OD2	2.45	0.50
1:A:536:PHE:HE1	1:A:590:GLY:HA3	1.75	0.50
1:A:879:SER:H	1:A:954:THR:HG22	1.76	0.50
1:A:904:ILE:HA	1:A:936:ALA:HB3	1.93	0.50
1:A:1397:TRP:NE1	1:A:1406:GLN:HB3	2.27	0.50
1:A:1414:ARG:NH1	1:A:1445:CYS:HA	2.26	0.50
1:A:1263:LYS:HG3	1:A:1265:SER:H	1.77	0.49
1:A:1469:THR:HG22	1:A:1481:GLN:HA	1.94	0.49
1:A:133:ASP:OD1	1:A:133:ASP:N	2.45	0.49
1:A:1514:TYR:CZ	1:A:1516:ILE:HD13	2.47	0.49
1:A:1569:GLY:N	1:A:1602:ASN:O	2.45	0.49
1:A:206:ARG:NH1	1:A:244:PRO:O	2.45	0.49
1:A:502:GLU:HB2	1:A:513:LYS:HB2	1.92	0.49
1:A:1012:THR:OG1	1:A:1031:THR:HB	2.13	0.49
1:A:1307:GLY:HA3	1:A:1371:GLY:O	2.12	0.49
1:A:1798:PRO:HG2	1:A:1801:PHE:HB2	1.93	0.49
1:A:630:VAL:HG23	1:A:632:PRO:HD3	1.95	0.49
1:A:1407:LYS:HZ2	1:A:1457:PHE:HD2	1.60	0.49
1:A:58:PRO:HG3	1:A:64:VAL:HG11	1.95	0.49
1:A:1022:PRO:HB2	1:A:1028:THR:HG21	1.94	0.49
1:A:540:ASP:OD1	1:A:541:THR:N	2.42	0.48
1:A:641:TYR:CG	1:A:716:LEU:HD22	2.48	0.48
1:A:1430:ASP:HB2	1:A:1432:VAL:HG12	1.95	0.48
1:A:956:VAL:HG13	1:A:1001:VAL:HG11	1.94	0.48
1:A:1055:TYR:CE1	1:A:1066:PRO:HD2	2.49	0.48
1:A:280:VAL:HG21	1:A:286:VAL:HG22	1.95	0.48
1:A:821:ILE:HG21	1:A:824:TYR:HD2	1.78	0.48
1:A:1285:LYS:HB3	1:A:1347:PHE:HE1	1.78	0.48
1:A:122:ILE:HG23	1:A:152:GLU:HA	1.95	0.48
1:A:365:ASP:OD1	1:A:365:ASP:N	2.44	0.48
1:A:301:ALA:HB1	1:A:336:THR:HA	1.95	0.48
1:A:890:ARG:HG2	1:A:893:ALA:N	2.26	0.48
1:A:1055:TYR:CB	1:A:1125:LYS:HG2	2.43	0.48
1:A:469:ASP:OD2	1:A:470:ARG:NH1	2.47	0.48
1:A:1242:ARG:HH21	1:A:1980:GLU:HB3	1.79	0.48
1:A:1469:THR:H	1:A:1542:LYS:HZ2	1.62	0.47
1:A:1047:GLY:CA	1:A:1101:MET:O	2.63	0.47
1:A:415:THR:HB	1:A:437:MET:HG3	1.95	0.47
1:A:497:LEU:HD11	1:A:516:PHE:HD2	1.79	0.47
1:A:1552:GLY:O	1:A:1566:CYS:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1712:ARG:O	1:A:1712:ARG:HD3	2.15	0.47
1:A:164:GLY:HA3	1:A:365:ASP:OD2	2.15	0.47
1:A:911:GLU:H	1:A:911:GLU:CD	2.18	0.47
1:A:1126:PHE:HB3	1:A:1147:VAL:HG23	1.96	0.47
1:A:1308:PHE:HB3	1:A:1317:CYS:HB2	1.95	0.47
1:A:1495:GLN:HA	1:A:1498:ALA:HB2	1.97	0.47
1:A:1589:ASP:OD1	1:A:1589:ASP:N	2.46	0.47
1:A:1015:PRO:HG2	1:A:1028:THR:HG22	1.96	0.47
1:A:186:ARG:NH1	1:A:215:ALA:O	2.45	0.47
1:A:351:TYR:CZ	1:A:357:LYS:HG3	2.49	0.47
1:A:389:LEU:HD23	1:A:486:VAL:HG23	1.97	0.47
1:A:420:TRP:CH2	1:A:433:THR:HG21	2.50	0.47
1:A:1469:THR:OG1	1:A:1542:LYS:NZ	2.26	0.47
1:A:1030:PHE:HZ	1:A:1116:TYR:HH	1.62	0.46
1:A:1292:PHE:CD2	1:A:1316:GLY:HA2	2.50	0.46
1:A:1033:THR:HA	1:A:1108:VAL:O	2.15	0.46
1:A:1321:SER:O	1:A:1324:THR:OG1	2.28	0.46
1:A:228:TYR:CZ	1:A:263:VAL:HG11	2.51	0.46
1:A:902:PRO:O	1:A:969:GLY:HA2	2.16	0.46
1:A:466:ARG:HD2	1:A:466:ARG:HA	1.72	0.46
1:A:1132:ALA:O	1:A:1135:THR:OG1	2.26	0.46
1:A:613:VAL:HB	1:A:654:PRO:HD2	1.98	0.46
1:A:1070:THR:HG23	1:A:1072:ALA:H	1.81	0.46
1:A:656:LEU:H	1:A:691:MET:HE2	1.81	0.46
1:A:1170:GLN:HG2	1:A:1171:ARG:H	1.81	0.46
1:A:1737:THR:HG22	1:A:1749:PRO:HG3	1.97	0.45
1:A:48:THR:OG1	1:A:69:THR:HB	2.17	0.45
1:A:1021:THR:HG23	1:A:1154:THR:O	2.15	0.45
1:A:1624:LEU:HD12	1:A:1625:PRO:CD	2.46	0.45
1:A:295:VAL:HG23	1:A:341:VAL:HG11	1.99	0.45
1:A:420:TRP:CD1	1:A:448:ILE:HD11	2.51	0.45
1:A:1398:SER:HB3	1:A:1405:CYS:HB2	1.97	0.45
1:A:1288:PRO:HD2	1:A:1291:TYR:CD1	2.51	0.45
1:A:1292:PHE:CD1	1:A:1304:CYS:HB3	2.52	0.45
1:A:764:ALA:HB3	1:A:859:THR:HG22	1.99	0.45
1:A:1647:ASN:O	1:A:1651:LEU:CA	2.65	0.45
1:A:86:GLY:N	1:A:119:TYR:OH	2.39	0.45
1:A:1055:TYR:HE2	1:A:1093:ASP:HB3	1.82	0.45
1:A:1847:LYS:HG3	1:A:1848:THR:HG22	1.98	0.45
1:A:643:ILE:HG13	1:A:698:ALA:HB3	1.98	0.45
1:A:649:VAL:HG23	1:A:696:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:PHE:HD2	1:A:1316:GLY:HA2	1.82	0.45
1:A:160:LEU:HB3	1:A:162:GLN:HE21	1.82	0.45
1:A:1016:ASN:HA	1:A:1022:PRO:HA	1.98	0.44
1:A:1413:TYR:HE2	1:A:1415:ASN:HB2	1.82	0.44
1:A:1508:PHE:N	1:A:1509:PRO:HD2	2.32	0.44
1:A:1920:PRO:HA	1:A:1921:PRO:HD2	1.92	0.44
1:A:212:ALA:HA	1:A:219:TYR:CZ	2.52	0.44
1:A:1097:ARG:HA	1:A:1097:ARG:HD3	1.76	0.44
1:A:150:TYR:HB3	1:A:249:LEU:HD23	2.00	0.44
1:A:289:THR:O	1:A:293:THR:HG23	2.17	0.44
1:A:1148:THR:O	1:A:1148:THR:OG1	2.32	0.44
1:A:81:PHE:HB2	1:A:129:LEU:HD11	1.99	0.44
1:A:876:VAL:HG13	1:A:1002:ALA:HB2	2.00	0.44
1:A:1101:MET:SD	1:A:1108:VAL:HB	2.58	0.44
1:A:777:ARG:HG2	1:A:779:ALA:H	1.83	0.44
1:A:1413:TYR:CE2	1:A:1415:ASN:HB2	2.53	0.44
1:A:1008:VAL:HA	1:A:1034:LEU:HB3	2.00	0.44
1:A:1072:ALA:HA	1:A:1075:LYS:NZ	2.32	0.44
1:A:1170:GLN:O	1:A:1172:VAL:HG23	2.17	0.44
1:A:1647:ASN:O	1:A:1651:LEU:HA	2.18	0.44
1:A:871:SER:HB3	1:A:883:THR:HB	1.99	0.43
1:A:1271:TYR:O	1:A:1274:VAL:HG22	2.18	0.43
1:A:1289:LYS:HZ3	1:A:1338:ALA:HA	1.84	0.43
1:A:192:THR:O	1:A:238:LEU:HA	2.19	0.43
1:A:1125:LYS:HE3	1:A:1127:PHE:HD2	1.82	0.43
1:A:1809:ARG:HA	1:A:1809:ARG:HD3	1.78	0.43
1:A:1239:GLU:OE2	1:A:1240:GLY:N	2.51	0.43
1:A:496:ALA:HB3	1:A:519:GLN:HB3	1.99	0.43
1:A:1192:ASN:HD22	1:A:1206:TYR:H	1.66	0.43
1:A:1421:GLN:HB2	1:A:1436:THR:OG1	2.19	0.43
1:A:1491:GLY:O	1:A:1496:GLN:NE2	2.49	0.43
1:A:877:LYS:HD2	1:A:877:LYS:HA	1.76	0.43
1:A:1634:THR:O	1:A:1672:GLN:NE2	2.51	0.43
1:A:788:LEU:HD23	1:A:788:LEU:HA	1.80	0.43
1:A:1247:CYS:SG	1:A:1248:PRO:HD2	2.59	0.43
1:A:1261:ARG:HB3	1:A:1266:ILE:HD11	2.00	0.42
1:A:275:VAL:CG1	1:A:288:PHE:HA	2.49	0.42
1:A:183:THR:O	1:A:186:ARG:NH1	2.52	0.42
1:A:639:TRP:CD1	1:A:714:PRO:HG2	2.55	0.42
1:A:1327:THR:HG23	1:A:1328:ASP:O	2.18	0.42
1:A:1485:GLY:HA2	1:A:1591:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD22	1:A:250:LEU:HD11	2.01	0.42
1:A:283:ALA:O	1:A:350:ARG:NH2	2.48	0.42
1:A:545:PRO:HB3	1:A:550:ALA:HB3	2.01	0.42
1:A:644:ILE:HG22	1:A:697:THR:CG2	2.46	0.42
1:A:772:ARG:HA	1:A:817:CYS:O	2.19	0.42
1:A:1058:GLN:HB2	1:A:1122:PHE:CE1	2.54	0.42
1:A:1270:THR:HG22	1:A:1271:TYR:H	1.84	0.42
1:A:523:ALA:HA	1:A:570:ILE:HB	2.01	0.42
1:A:1398:SER:HB3	1:A:1405:CYS:CB	2.50	0.42
1:A:1634:THR:N	1:A:1672:GLN:HE22	2.18	0.42
1:A:1724:ARG:NE	1:A:1724:ARG:HA	2.34	0.42
1:A:1968:ALA:O	1:A:1971:GLU:HG2	2.19	0.42
1:A:350:ARG:HH21	1:A:470:ARG:NH1	2.18	0.42
1:A:476:ASN:OD1	1:A:476:ASN:N	2.52	0.42
1:A:1126:PHE:H	1:A:1147:VAL:HG21	1.85	0.42
1:A:1469:THR:O	1:A:1542:LYS:HD2	2.20	0.42
1:A:1719:MET:CE	1:A:1719:MET:HA	2.50	0.42
1:A:439:ASN:OD1	1:A:439:ASN:N	2.53	0.42
1:A:522:LYS:HE3	1:A:522:LYS:HB3	1.87	0.42
1:A:588:LEU:HD21	1:A:612:GLN:HA	2.01	0.42
1:A:216:SER:O	1:A:216:SER:OG	2.36	0.41
1:A:1503:ASN:ND2	1:A:1507:ASP:H	2.18	0.41
1:A:167:ARG:HD3	1:A:168:LEU:N	2.35	0.41
1:A:944:THR:O	1:A:944:THR:OG1	2.38	0.41
1:A:1286:LYS:NZ	1:A:1313:GLY:HA3	2.35	0.41
1:A:1329:GLY:HA3	1:A:1357:THR:HG21	2.00	0.41
1:A:421:THR:HB	1:A:428:GLU:HB2	2.02	0.41
1:A:1237:SER:HB3	1:A:1244:CYS:SG	2.60	0.41
1:A:54:PRO:HB2	1:A:56:VAL:HG12	2.02	0.41
1:A:719:ILE:HD11	1:A:729:THR:H	1.86	0.41
1:A:1058:GLN:HB2	1:A:1122:PHE:HE1	1.85	0.41
1:A:1715:LYS:H	1:A:1715:LYS:HG3	1.67	0.41
1:A:44:THR:N	1:A:74:ASP:OD2	2.48	0.41
1:A:466:ARG:CZ	1:A:480:LEU:HA	2.51	0.41
1:A:536:PHE:HB3	1:A:577:PHE:CE2	2.55	0.41
1:A:1071:ASP:OD1	1:A:1071:ASP:N	2.53	0.41
1:A:1604:GLU:OE2	1:A:1607:GLN:HG2	2.20	0.41
1:A:515:SER:HB2	1:A:517:ARG:HH12	1.86	0.41
1:A:619:THR:HG23	1:A:645:ARG:HB3	2.01	0.41
1:A:403:ILE:HD13	1:A:403:ILE:HA	1.94	0.41
1:A:483:SER:O	1:A:484:THR:OG1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HD3	1:A:221:PHE:O	2.20	0.41
1:A:902:PRO:O	1:A:902:PRO:HD2	2.21	0.41
1:A:1082:THR:O	1:A:1082:THR:OG1	2.35	0.41
1:A:1277:LEU:HD23	1:A:1277:LEU:HA	1.82	0.41
1:A:1415:ASN:ND2	1:A:1460:SER:O	2.51	0.41
1:A:1506:ASN:ND2	1:A:1508:PHE:H	2.19	0.41
1:A:1652:ILE:HG22	1:A:1654:THR:HG23	2.02	0.41
1:A:71:ALA:HA	1:A:103:THR:HA	2.02	0.41
1:A:866:VAL:HG13	1:A:888:ILE:HG13	2.03	0.41
1:A:1374:ALA:HA	1:A:1388:PRO:HD3	2.02	0.41
1:A:1424:SER:HB3	1:A:1427:ILE:HD12	2.03	0.41
1:A:1567:LYS:O	1:A:1570:THR:OG1	2.24	0.41
1:A:1632:PRO:HB2	1:A:1695:ALA:HA	2.02	0.41
1:A:1704:ARG:HA	1:A:1716:PRO:HA	2.02	0.41
1:A:1845:LYS:O	1:A:1847:LYS:N	2.53	0.40
1:A:471:ASP:HB2	1:A:473:VAL:HG23	2.04	0.40
1:A:1193:ASP:HB3	1:A:1202:ALA:O	2.21	0.40
1:A:1688:TYR:HB2	1:A:1712:ARG:NH1	2.36	0.40
1:A:1661:GLN:HA	1:A:1661:GLN:OE1	2.22	0.40
1:A:1830:GLU:HB2	1:A:1838:LYS:HG3	2.02	0.40
1:A:188:ASP:HB2	1:A:190:TRP:CZ2	2.57	0.40
1:A:328:LEU:HD12	1:A:328:LEU:HA	1.83	0.40
1:A:365:ASP:OD1	1:A:369:ASN:HB3	2.22	0.40
1:A:752:THR:HG22	1:A:776:THR:HB	2.03	0.40
1:A:266:PRO:O	1:A:269:TYR:HB2	2.21	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	1884/1987 (95%)	1756 (93%)	124 (7%)	4 (0%)	47 79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	VAL
1	A	1143	VAL
1	A	613	VAL
1	A	1939	PRO

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	1488/1571 (95%)	1446 (97%)	42 (3%)	43 72

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	66	PHE
1	A	119	TYR
1	A	125	LYS
1	A	205	SER
1	A	242	ASP
1	A	483	SER
1	A	534	CYS
1	A	536	PHE
1	A	547	ASP
1	A	579	ARG
1	A	603	ASP
1	A	726	ASP
1	A	800	SER
1	A	817	CYS
1	A	824	TYR
1	A	938	MET
1	A	995	PHE
1	A	1017	TYR
1	A	1061	ASN
1	A	1064	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1089	ASN
1	A	1131	TYR
1	A	1176	LYS
1	A	1183	PHE
1	A	1195	TYR
1	A	1273	PHE
1	A	1292	PHE
1	A	1295	ASN
1	A	1301	CYS
1	A	1361	CYS
1	A	1377	SER
1	A	1453	TYR
1	A	1463	LEU
1	A	1543	SER
1	A	1697	CYS
1	A	1746	GLN
1	A	1747	CYS
1	A	1750	CYS
1	A	1799	TYR
1	A	1871	ARG
1	A	1891	ASN

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	57	ASN
1	A	1506	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 monosaccharides 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.

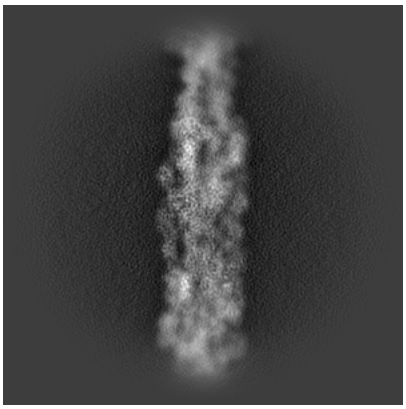
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41674. These allow visual inspection of the internal detail of the map and identification of artifacts.

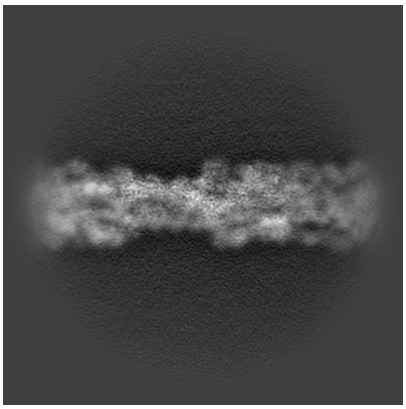
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

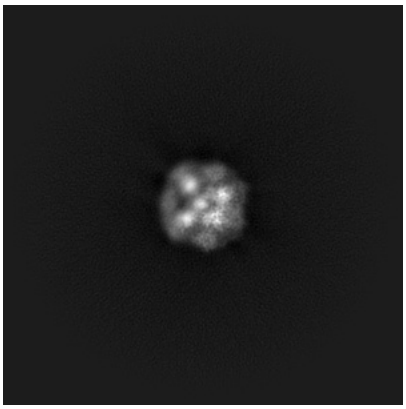
6.1.1 Primary map



X

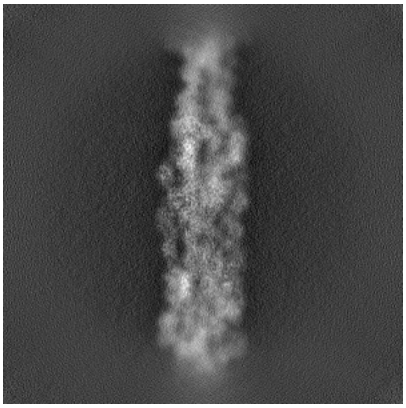


Y

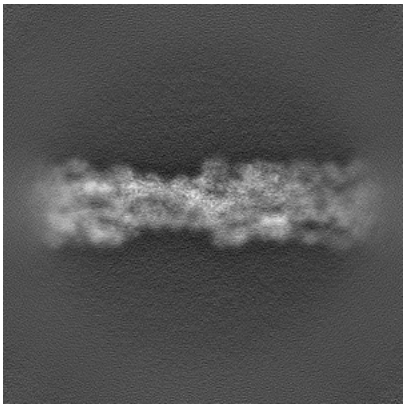


Z

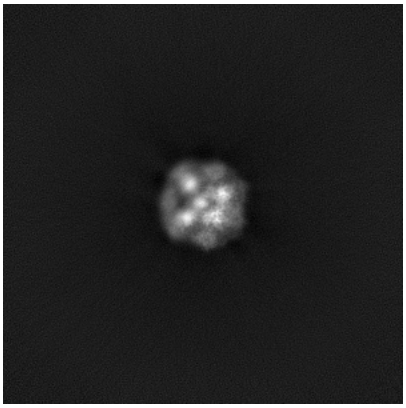
6.1.2 Raw map



X



Y

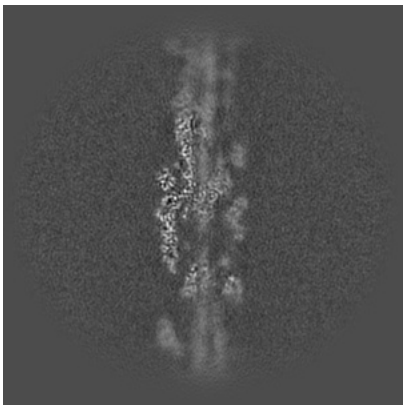


Z

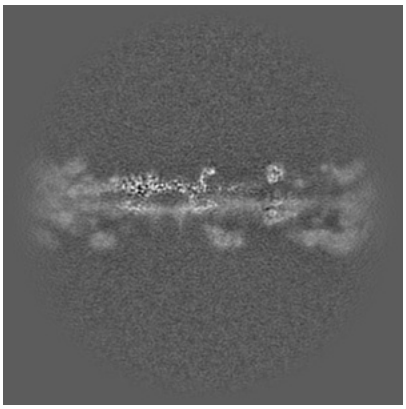
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

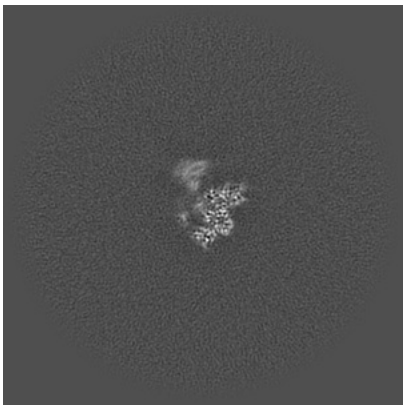
6.2.1 Primary map



X Index: 186

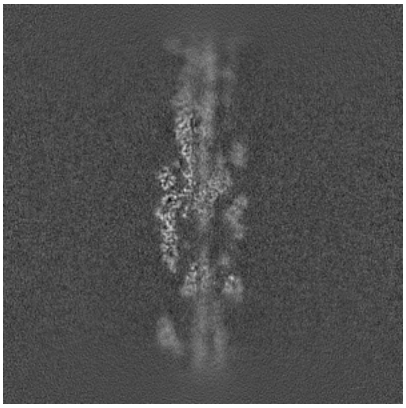


Y Index: 186

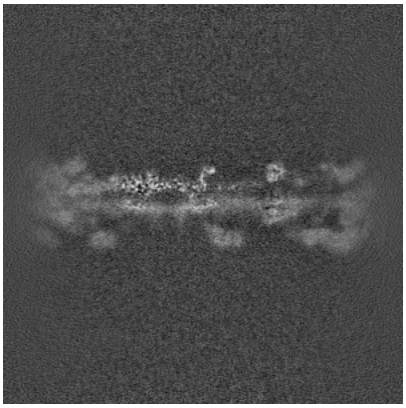


Z Index: 186

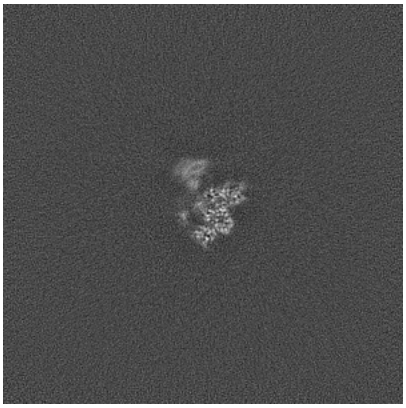
6.2.2 Raw map



X Index: 186



Y Index: 186

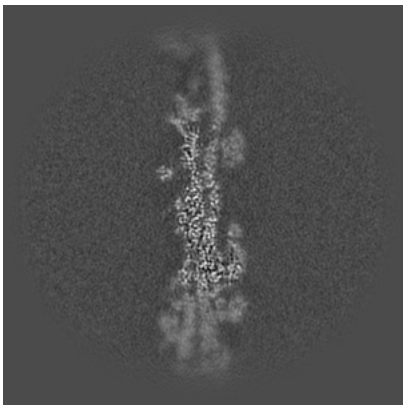


Z Index: 186

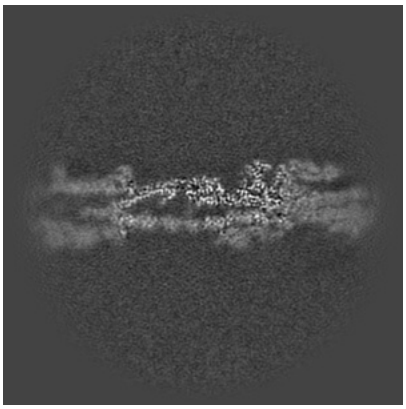
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



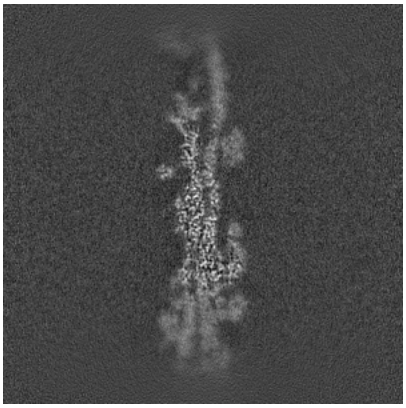
X Index: 202



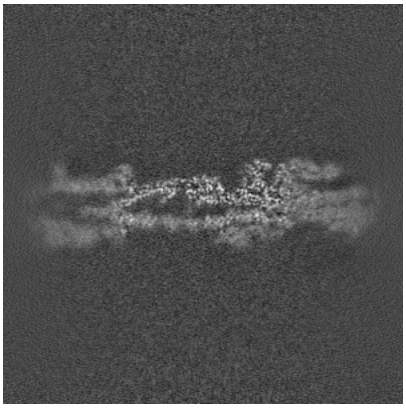
Y Index: 171

Z Index: 194

6.3.2 Raw map



X Index: 202



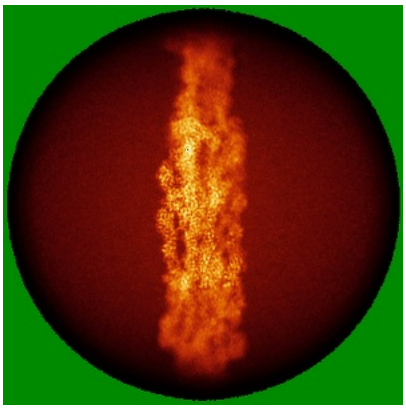
Y Index: 171

Z Index: 194

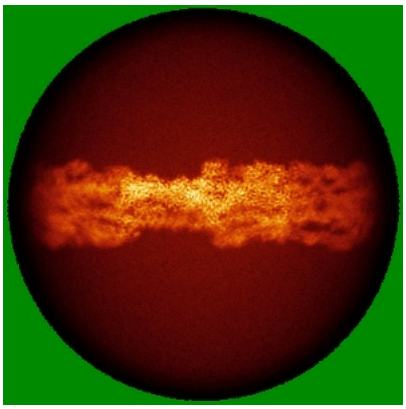
The images above show the largest variance slices of the map in three orthogonal directions.

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

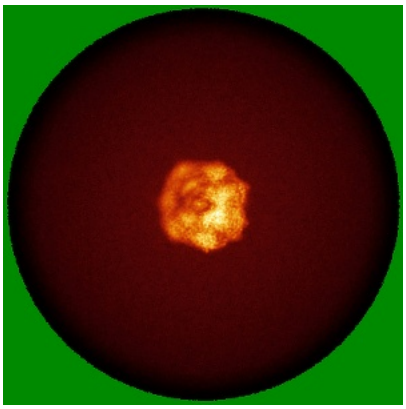
6.4.1 Primary map



X

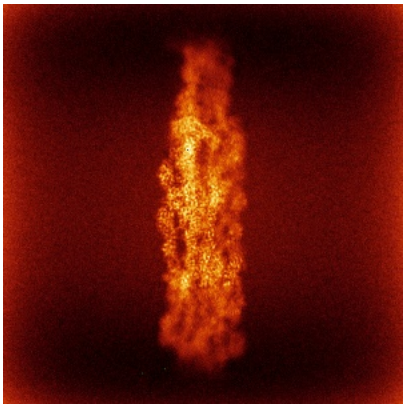


Y

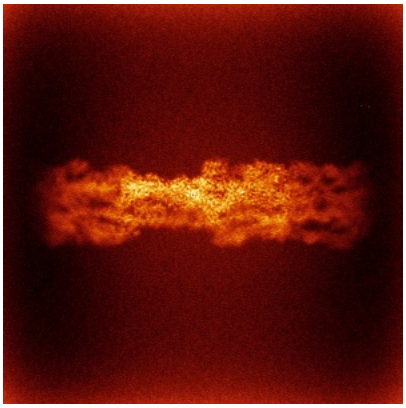


Z

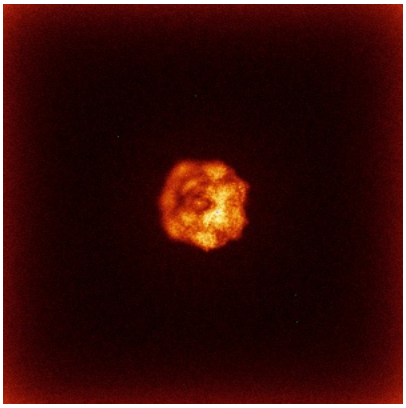
6.4.2 Raw map



X



Y

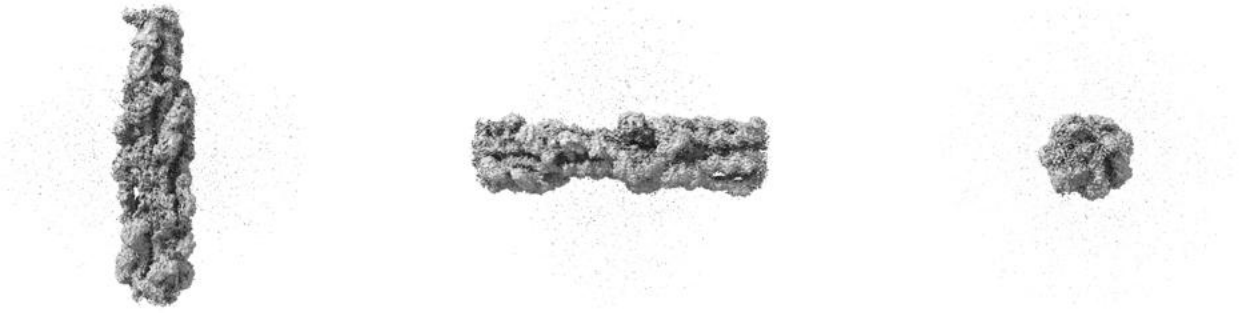


Z

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)

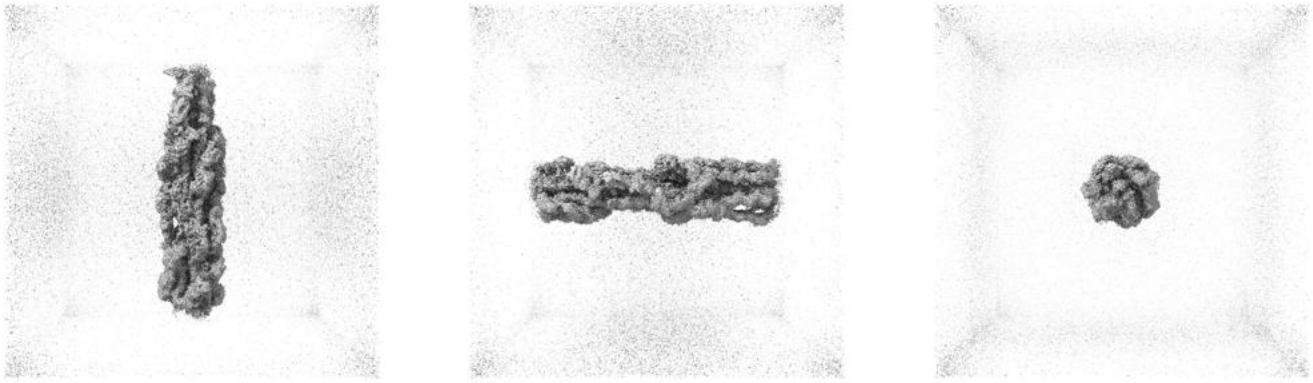
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.321. 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.

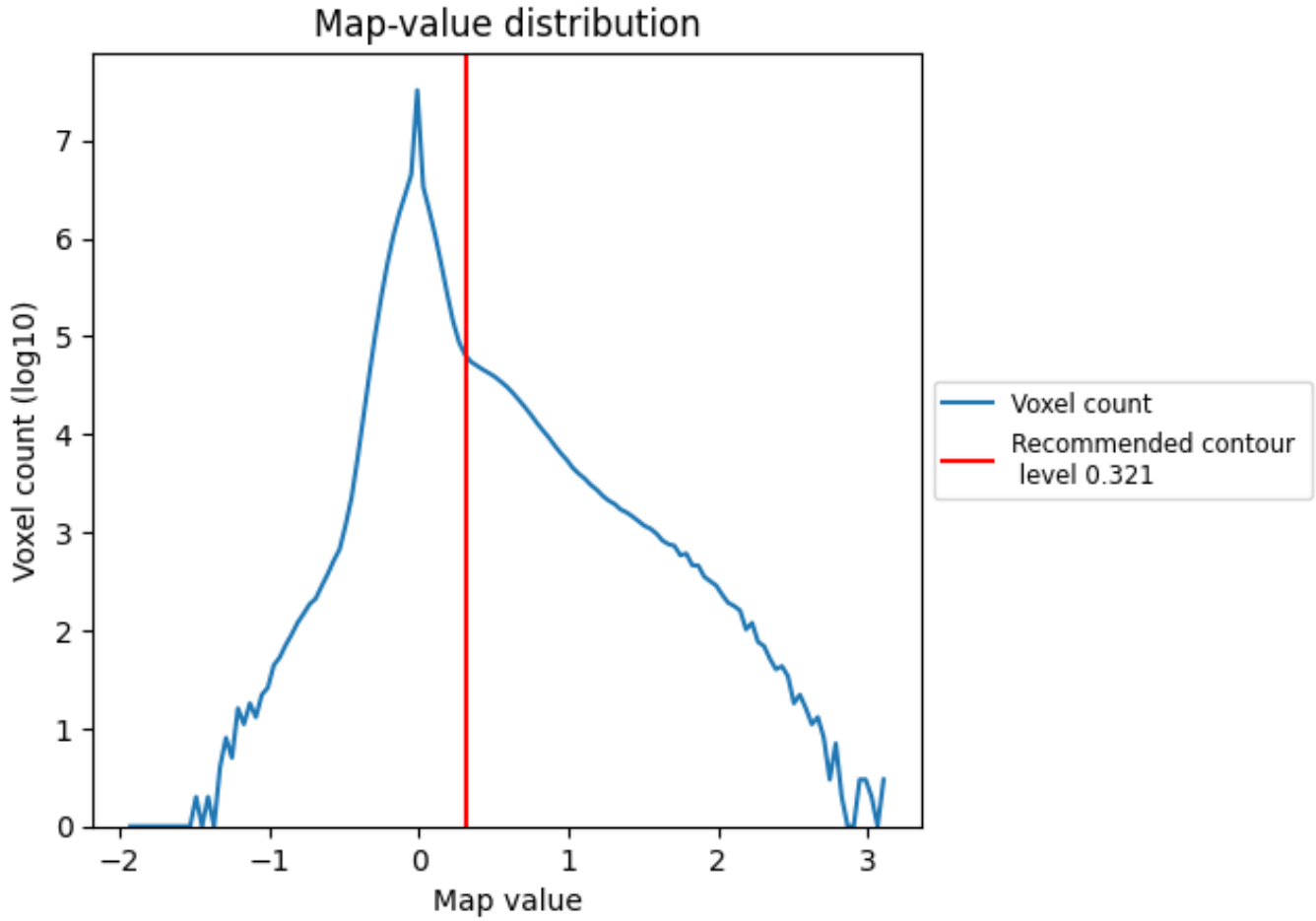
6.6 Mask visualisation (i)

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

7 Map analysis

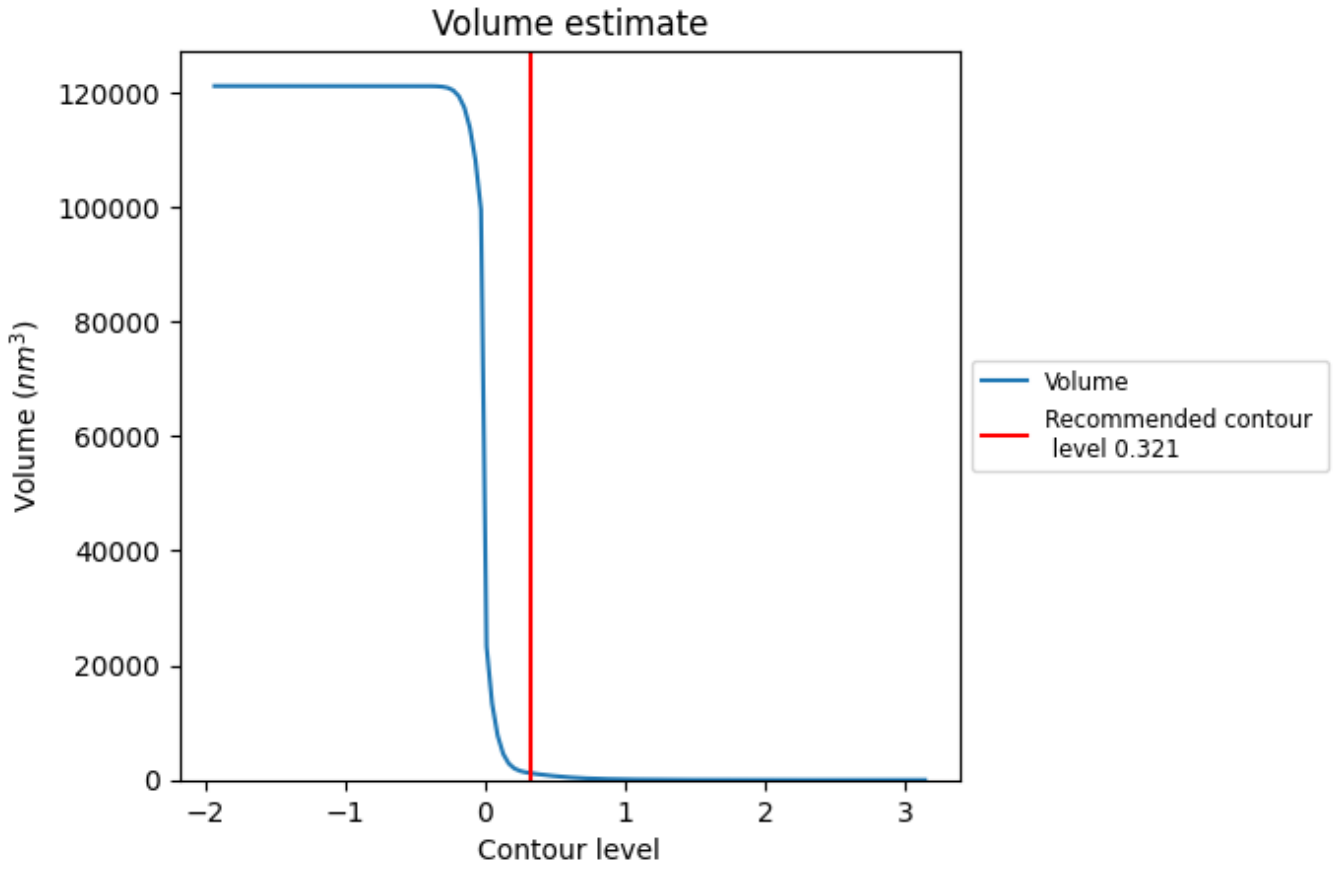
This section contains the results of statistical analysis of the map.

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.

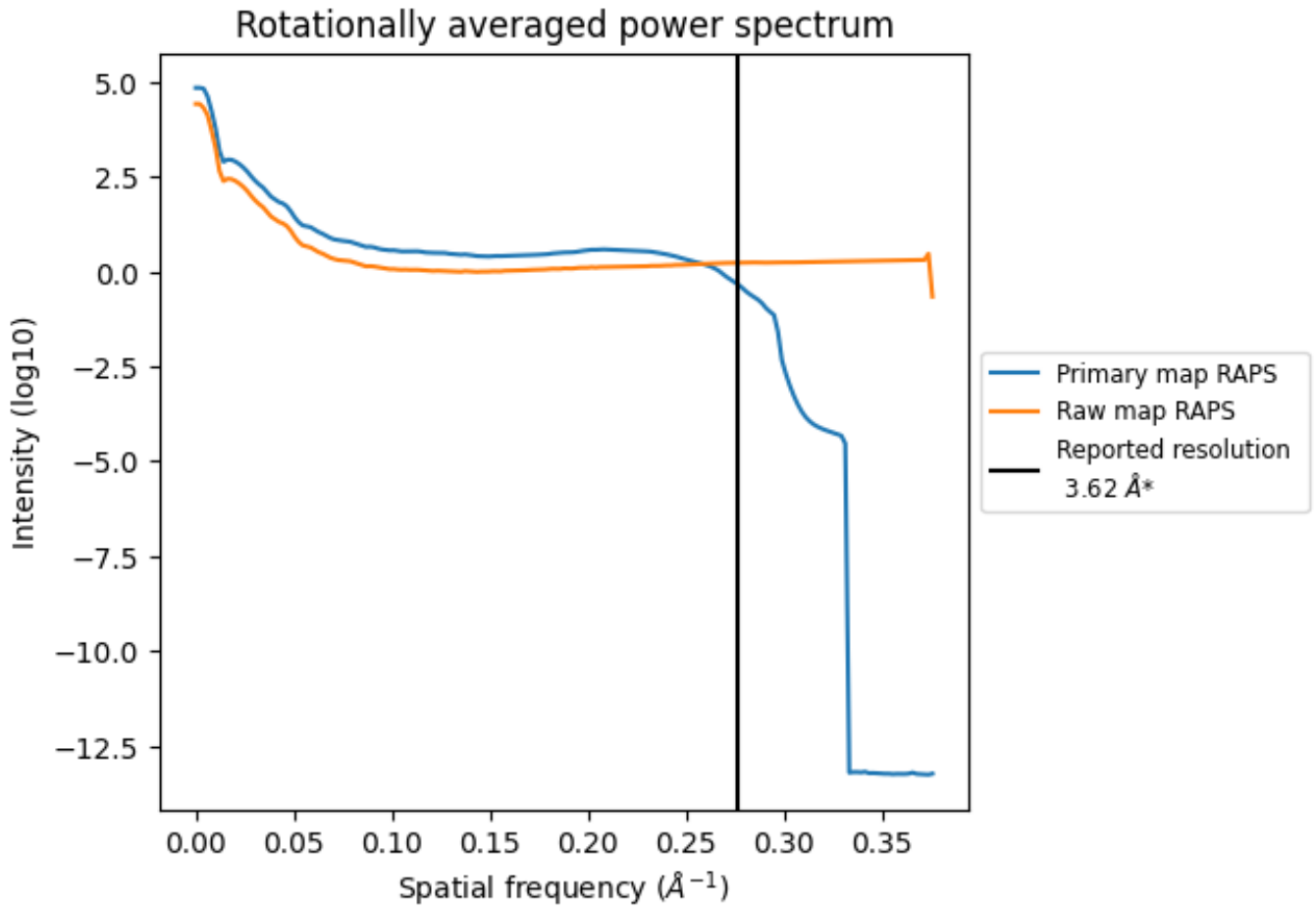
7.2 Volume estimate



The volume at the recommended contour level is 1211 nm^3; this corresponds to an approximate mass of 1094 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)

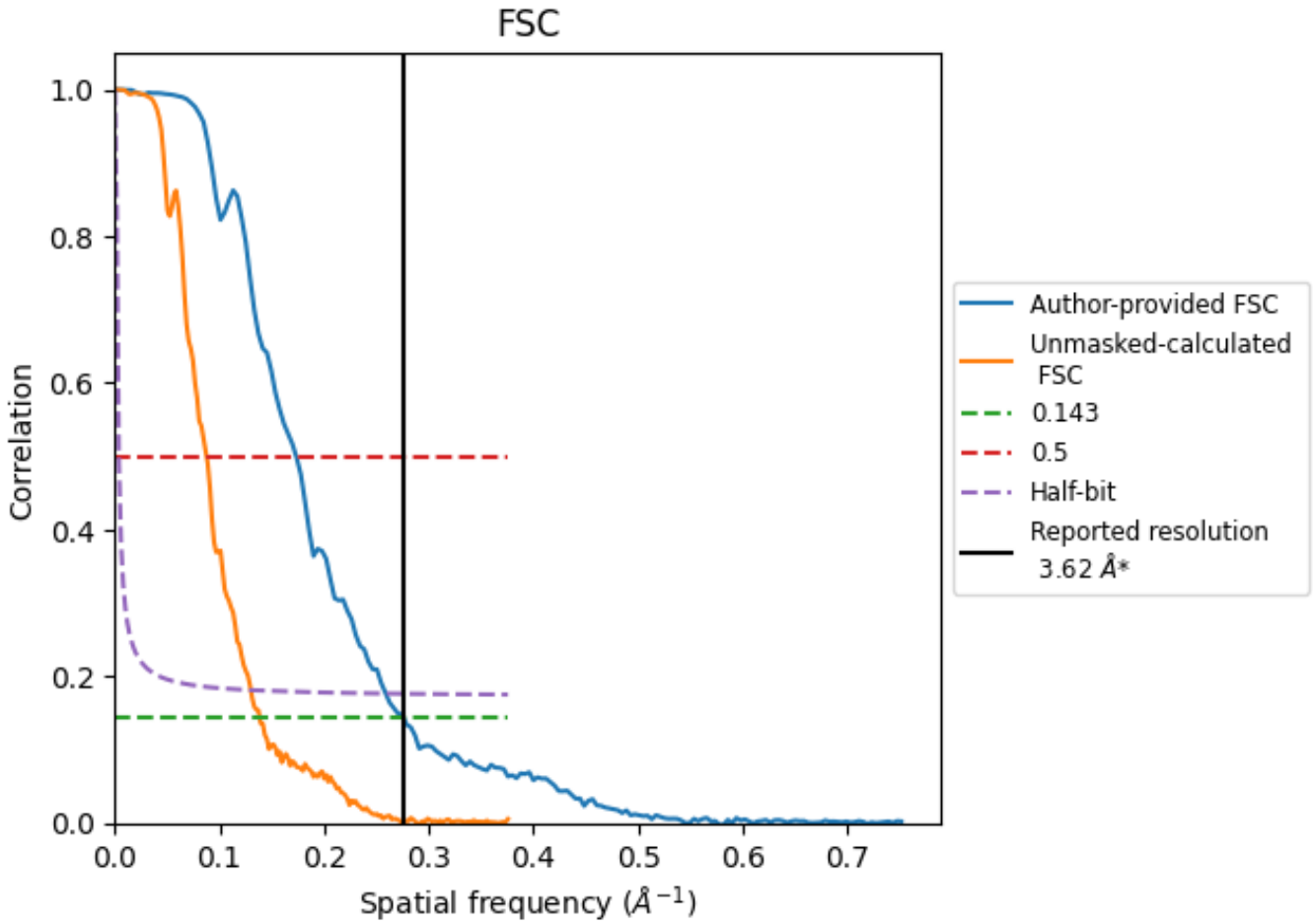


*Reported resolution corresponds to spatial frequency of 0.276 Å^{-1}

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 0.276 Å^{-1}

8.2 Resolution estimates (i)

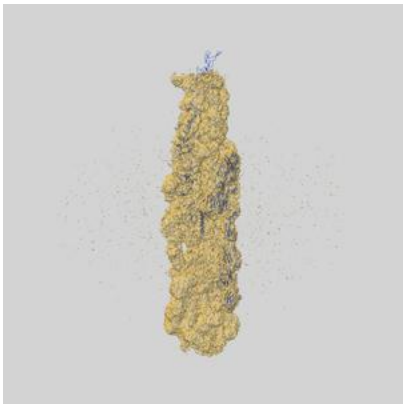
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.62	5.77	3.88
Unmasked-calculated*	7.22	11.39	7.69

*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 7.22 differs from the reported value 3.62 by more than 10 %

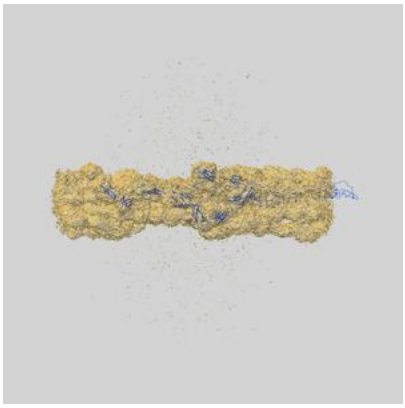
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41674 and PDB model 8TX1. Per-residue inclusion information can be found in section 3 on page 5.

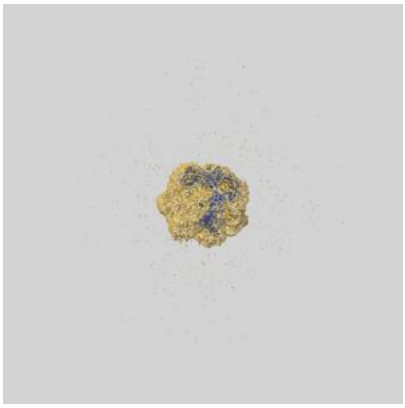
9.1 Map-model overlay



X



Y



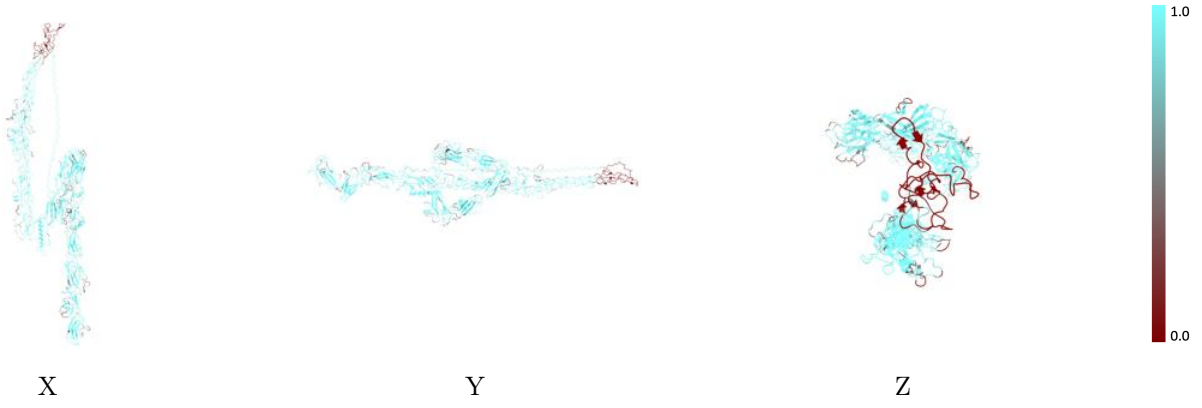
Z

The images above show the 3D surface view of the map at the recommended contour level 0.321 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)

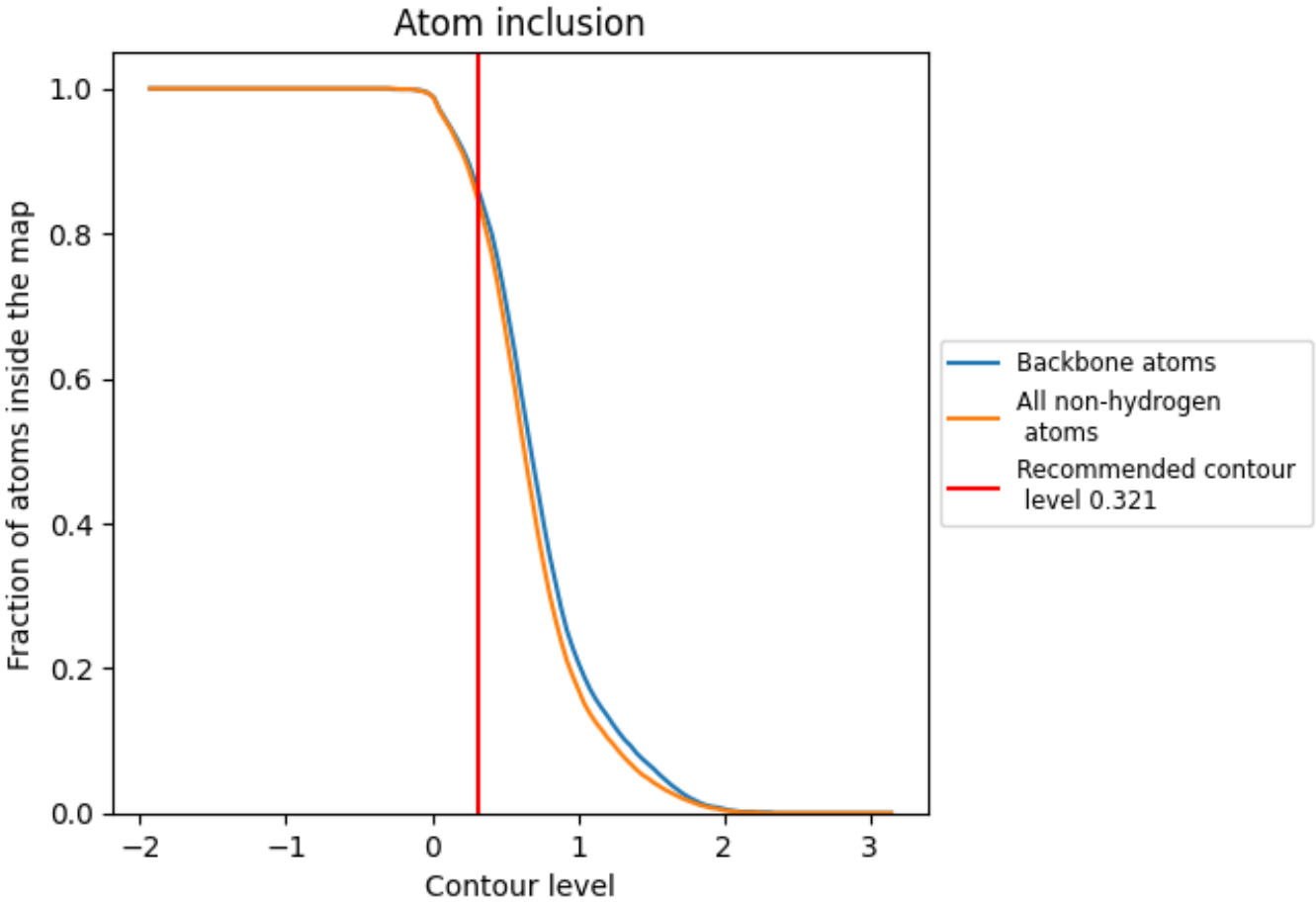
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.321).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.321) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.2200
A	0.8420	0.2200