Full wwPDB EM Validation Report ⓘ

Mar 12, 2024 – 12:39 pm GMT

PDB ID	:	8QEO
EMDB ID	:	EMD-18374
Title	:	cryo-EM structure complex of Frizzled-7 and Clostridioides difficile toxin B
Authors	:	Kinsolving, J.; Bous, J.
Deposited on	:	2023-09-01
Resolution	:	3.26 Å(reported)
Based on initial model	:	.

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:

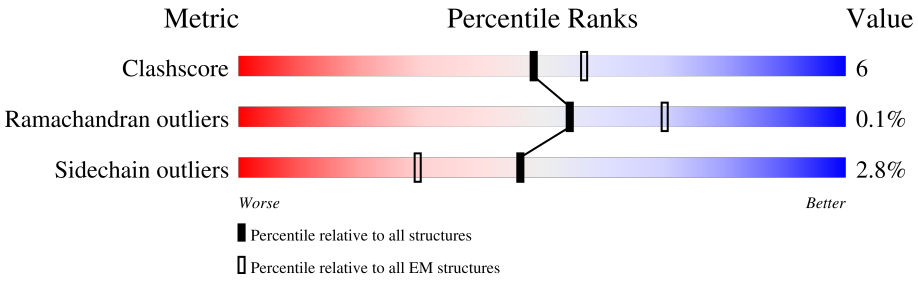
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.26 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	2397	24% 74% 15% · 10%
2	B	603	11% 16% · 80%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18126 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 Toxin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2146	17176	10943	2710	3477	46	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P18177
A	-12	ASP	-	expression tag	UNP P18177
A	-11	LYS	-	expression tag	UNP P18177
A	-10	LEU	-	expression tag	UNP P18177
A	-9	VAL	-	expression tag	UNP P18177
A	-8	HIS	-	expression tag	UNP P18177
A	-7	LEU	-	expression tag	UNP P18177
A	-6	ASN	-	expression tag	UNP P18177
A	-5	GLN	-	expression tag	UNP P18177
A	-4	ARG	-	expression tag	UNP P18177
A	-3	GLY	-	expression tag	UNP P18177
A	-2	LYS	-	expression tag	UNP P18177
A	-1	CYS	-	expression tag	UNP P18177
A	0	THR	-	expression tag	UNP P18177
A	2367	GLY	-	expression tag	UNP P18177
A	2368	TYR	-	expression tag	UNP P18177
A	2369	ARG	-	expression tag	UNP P18177
A	2370	PRO	-	expression tag	UNP P18177
A	2371	HIS	-	expression tag	UNP P18177
A	2372	ALA	-	expression tag	UNP P18177
A	2373	GLY	-	expression tag	UNP P18177
A	2374	LEU	-	expression tag	UNP P18177
A	2375	ARG	-	expression tag	UNP P18177
A	2376	GLY	-	expression tag	UNP P18177
A	2377	SER	-	expression tag	UNP P18177
A	2378	HIS	-	expression tag	UNP P18177
A	2379	HIS	-	expression tag	UNP P18177
A	2380	HIS	-	expression tag	UNP P18177

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2381	HIS	-	expression tag	UNP P18177
A	2382	HIS	-	expression tag	UNP P18177
A	2383	HIS	-	expression tag	UNP P18177

- Molecule 2 is a protein called Frizzled-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	S	0	0
			949	600	165	172	12		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	MET	-	initiating methionine	UNP O75084
B	11	LYS	-	expression tag	UNP O75084
B	12	THR	-	expression tag	UNP O75084
B	13	ILE	-	expression tag	UNP O75084
B	14	ILE	-	expression tag	UNP O75084
B	15	ALA	-	expression tag	UNP O75084
B	16	LEU	-	expression tag	UNP O75084
B	17	SER	-	expression tag	UNP O75084
B	18	TYR	-	expression tag	UNP O75084
B	19	ILE	-	expression tag	UNP O75084
B	20	PHE	-	expression tag	UNP O75084
B	21	CYS	-	expression tag	UNP O75084
B	22	LEU	-	expression tag	UNP O75084
B	23	VAL	-	expression tag	UNP O75084
B	24	PHE	-	expression tag	UNP O75084
B	25	ALA	-	expression tag	UNP O75084
B	26	ASP	-	expression tag	UNP O75084
B	27	TYR	-	expression tag	UNP O75084
B	28	LYS	-	expression tag	UNP O75084
B	29	ASP	-	expression tag	UNP O75084
B	30	ASP	-	expression tag	UNP O75084
B	31	ASP	-	expression tag	UNP O75084
B	32	ASP	-	expression tag	UNP O75084
B	575	SER	-	expression tag	UNP O75084
B	576	ARG	-	expression tag	UNP O75084
B	577	LEU	-	expression tag	UNP O75084
B	578	GLU	-	expression tag	UNP O75084
B	579	VAL	-	expression tag	UNP O75084
B	580	LEU	-	expression tag	UNP O75084

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Chain	Residue	Modelled	Actual	Comment	Reference
B	581	PHE	-	expression tag	UNP O75084
B	582	GLN	-	expression tag	UNP O75084
B	583	GLY	-	expression tag	UNP O75084
B	584	PRO	-	expression tag	UNP O75084
B	585	TRP	-	expression tag	UNP O75084
B	586	SER	-	expression tag	UNP O75084
B	587	HIS	-	expression tag	UNP O75084
B	588	PRO	-	expression tag	UNP O75084
B	589	GLN	-	expression tag	UNP O75084
B	590	PHE	-	expression tag	UNP O75084
B	591	GLU	-	expression tag	UNP O75084
B	592	LYS	-	expression tag	UNP O75084
B	593	GLY	-	expression tag	UNP O75084
B	594	GLY	-	expression tag	UNP O75084
B	595	GLY	-	expression tag	UNP O75084
B	596	SER	-	expression tag	UNP O75084
B	597	GLY	-	expression tag	UNP O75084
B	598	GLY	-	expression tag	UNP O75084
B	599	GLY	-	expression tag	UNP O75084
B	600	SER	-	expression tag	UNP O75084
B	601	GLY	-	expression tag	UNP O75084
B	602	GLY	-	expression tag	UNP O75084
B	603	GLY	-	expression tag	UNP O75084
B	604	SER	-	expression tag	UNP O75084
B	605	TRP	-	expression tag	UNP O75084
B	606	SER	-	expression tag	UNP O75084
B	607	HIS	-	expression tag	UNP O75084
B	608	PRO	-	expression tag	UNP O75084
B	609	GLN	-	expression tag	UNP O75084
B	610	PHE	-	expression tag	UNP O75084
B	611	GLU	-	expression tag	UNP O75084
B	612	LYS	-	expression tag	UNP O75084

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

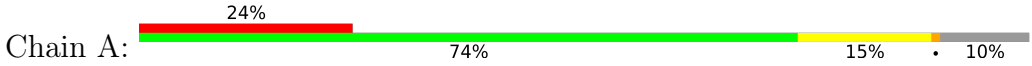
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0

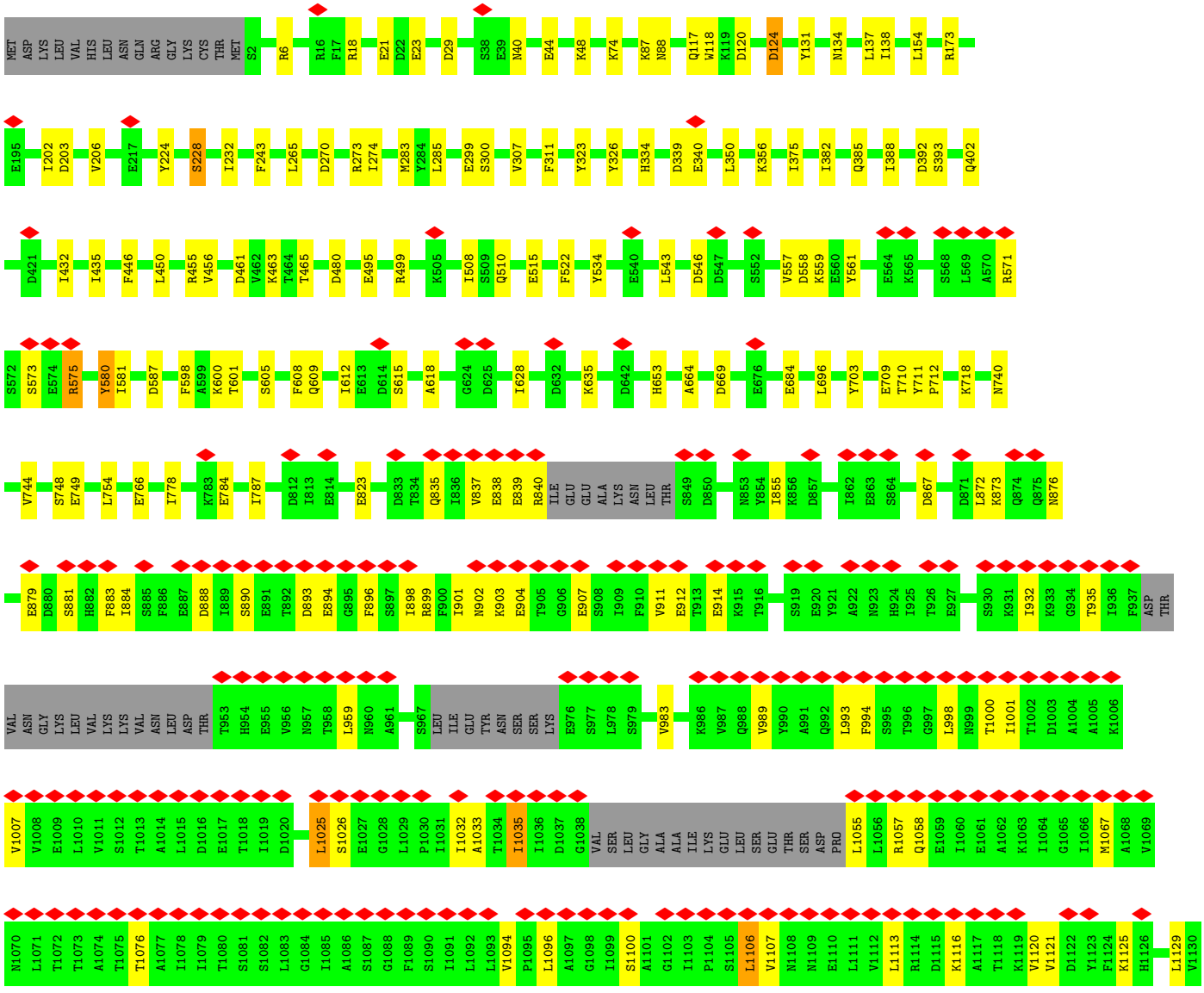
3 Residue-property plots (i)

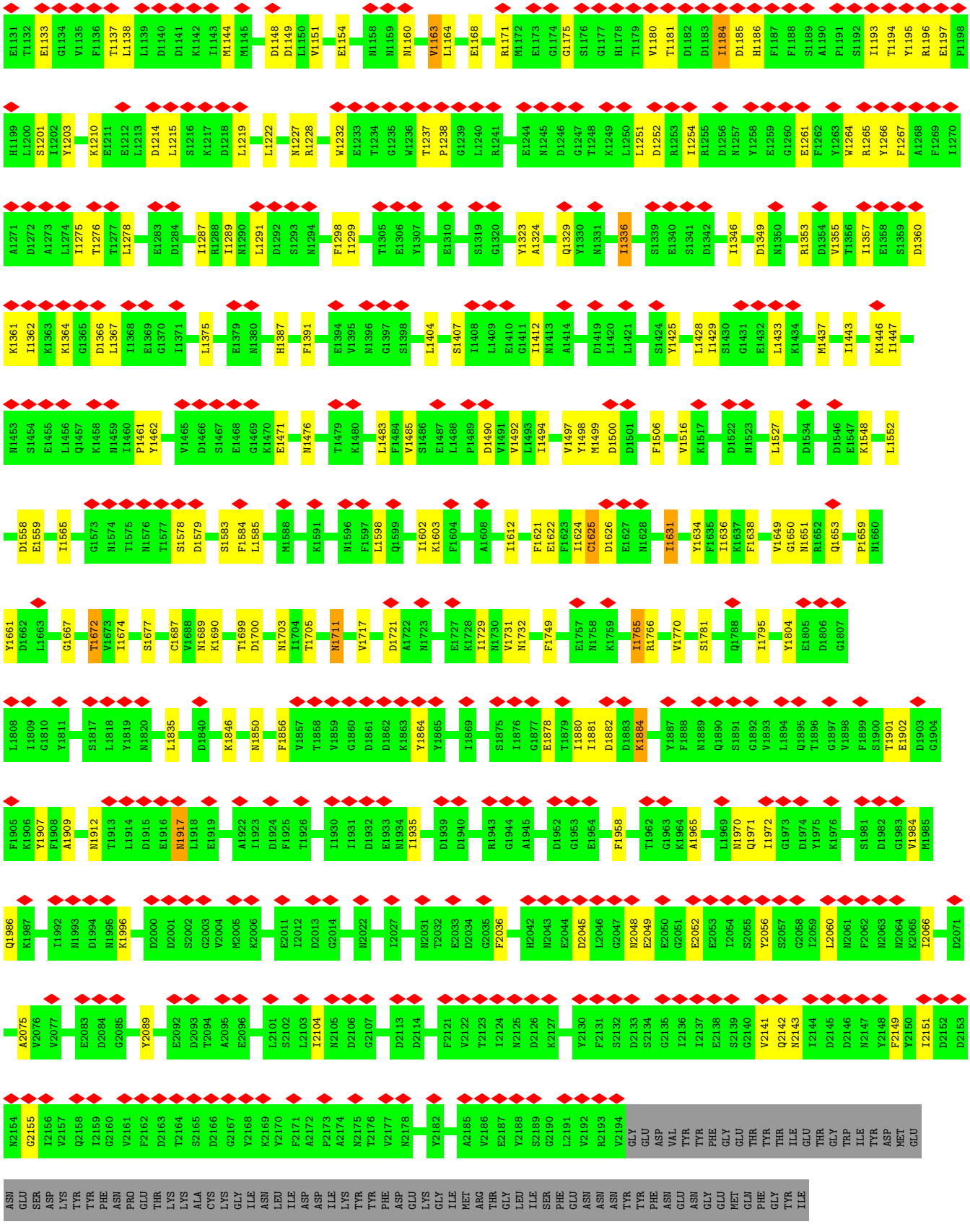
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

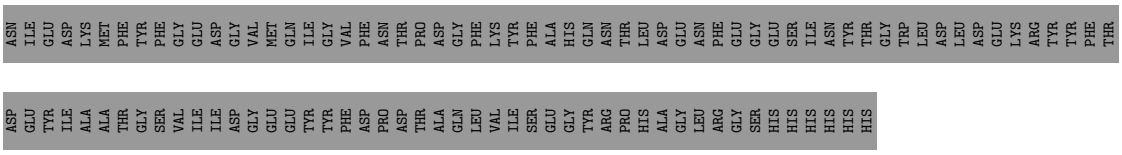
- Molecule 1: Toxin B

Chain A:



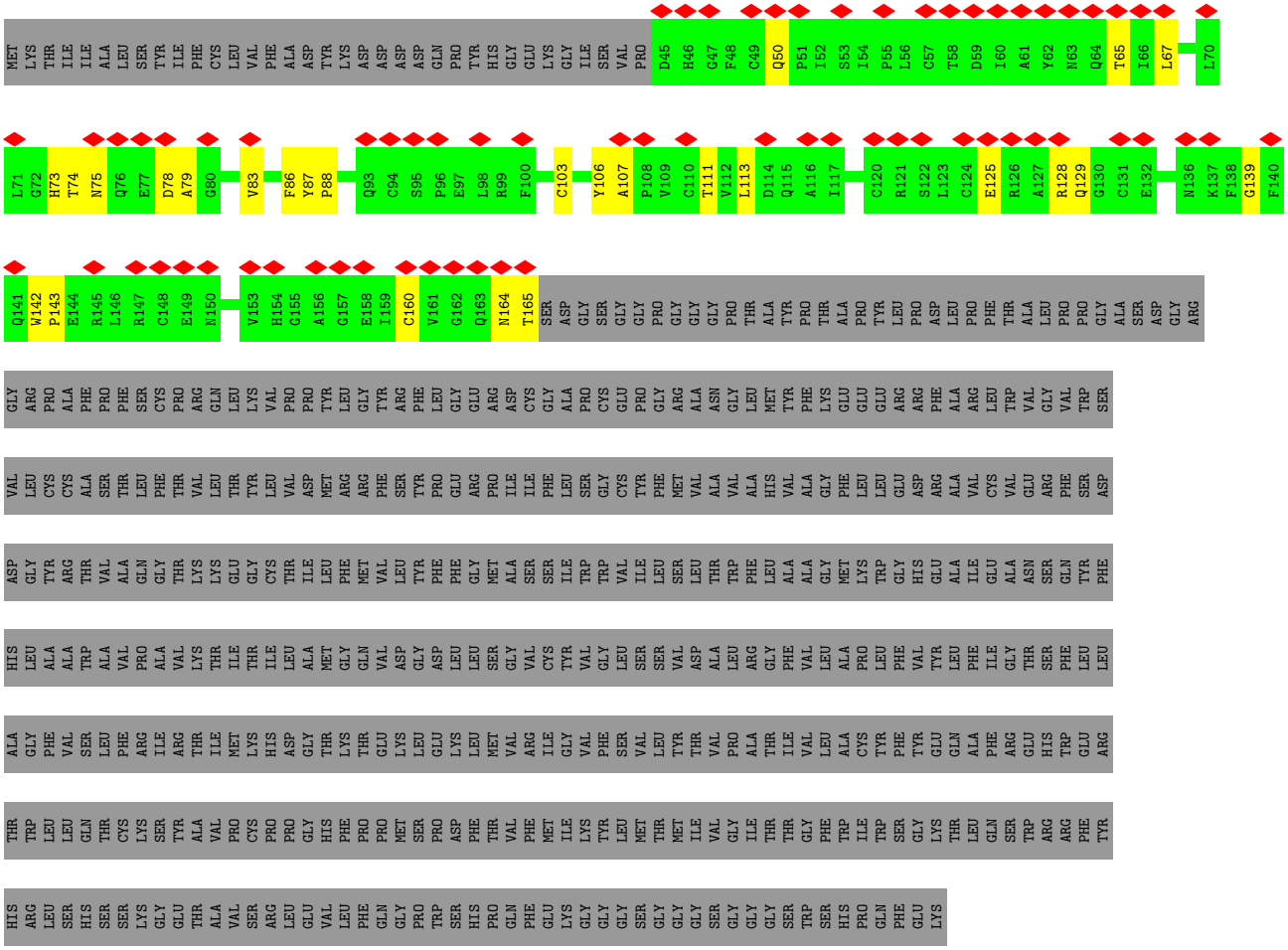



E1131 T1132 E1133 G1134 V1135 F1136 T1137 L1138 L1139 D1140 D1141 K1142 I1143 M1144 M1145 D1148 D1149 L1150 V1151 E1154 N1158 N1159 N1160 V1163 L1164 E1168 R1171 M1172 E1173 G1174 G1175 S1176 G1177 H1178 T1179 V1180 T1181 D1182 D1183 I1184 D1185 H1186 F1187 F1188 S1189 A1190 P1191 S1192 I1193 T1194 Y1195 R1196 E1197 P1198
H1199 L1200 S1201 I1202 Y1203 K1210 E1211 E1212 L1213 D1214 L1215 S1216 K1217 D1218 L1219 L1222 N1227 R1228 W1232 E1233 T1234 G1235 W1236 T1237 P1238 G1239 L1240 R1241 E1244 N1245 D1246 G1247 T1248 K1249 L1250 L1251 D1252 R1253 I1254 R1255 D1256 N1257 Y1258 E1259 G1260 E1261 F1262 Y1263 W1264 R1265 Y1266 F1267 A1268 F1269 I1270
A1271 D1272 A1273 L1274 I1275 T1276 T1277 L1278 E1283 D1284 I1287 R1288 I1289 N1290 L1291 D1292 S1293 N1294 F1298 I1299 T1305 E1306 Y1307 E1310 S1319 G1320 Y1323 A1324 Q1329 Y1330 N1331 I1336 S1339 E1340 S1341 D1342 I1346 D1349 N1350 R1353 D1354 V1355 T1356 I1357 E1358 S1359 D1360
K1361 I1362 K1363 K1364 G1365 D1366 L1367 I1368 E1369 G1370 I1371 L1375 E1379 N1380 H1387 F1391 E1394 V1395 N1396 G1397 S1398 L1404 S1407 I1408 L1409 E1410 G1411 I1412 N1413 A1414 D1419 L1420 L1421 S1424 Y1425 L1428 I1429 S1430 G1431 E1432 L1433 K1434 M1437 I1443 K1446 I1447
N1453 S1454 E1455 L1456 Q1457 K1458 N1459 I1460 P1461 Y1462 V1465 D1466 S1467 E1468 G1469 K1470 E1471 N1476 T1479 K1480 L1483 F1484 V1485 S1486 E1487 L1488 P1489 D1490 V1491 V1492 L1493 I1494 V1497 Y1498 M1499 D1500 D1501 F1506 V1516 K1517 D1522 N1523 L1527 D1534 D1546 E1547 K1548 L1552
D1558 E1559 I1565 G1573 N1574 T1575 N1576 T1577 S1578 D1579 S1583 F1584 L1585 M1588 K1591 N1596 F1597 L1598 Q1599 I1602 K1603 F1604 A1608 I1612 F1621 E1622 F1623 I1624 C1625 D1626 E1627 N1628 I1631 Y1634 F1635 I1636 K1637 F1638 V1649 G1650 N1651 R1652 Q1653 P1659 N1660
Y1661 D1662 L1663 G1667 T1672 Y1673 I1674 S1677 C1687 Y1688 N1689 K1690 T1699 D1700 N1703 I1704 T1705 N1711 V1717 D1721 A1722 N1723 E1727 K1728 I1729 N1730 V1731 N1732 F1749 E1757 N1758 K1759 I1765 R1766 V1770 S1781 Q1788 I1795 Y1804 E1805 D1806 G1807
L1808 I1809 G1810 Y1811 S1817 L1818 Y1819 N1820 L1835 D1840 K1846 N1850 F1856 V1857 T1858 V1859 G1860 D1861 D1862 K1863 Y1864 Y1865 I1869 S1875 I1876 G1877 E1878 T1879 I1880 I1881 D1882 D1883 K1884 Y1887 F1888 N1889 Q1890 S1891 G1892 V1893 L1894 Q1895 T1896 G1897 V1898 F1899 S1900 T1901 E1902 D1903 G1904
F1905 K1906 Y1907 F1908 A1909 N1912 T1913 L1914 D1915 E1916 N1917 L1918 E1919 A1922 I1923 D1924 F1925 T1926 I1930 I1931 D1932 E1933 N1934 I1935 D1939 D1940 R1943 G1944 A1945 D1952 G1953 E1954 F1958 T1962 G1963 K1964 A1965 L1969 N1970 Q1971 I1972 G1973 D1974 Y1975 K1976 S1981 D1982 G1983 V1984 M1985
Q1986 K1987 I1992 N1993 D1994 N1995 K1996 D2000 D2001 S2002 G2003 V2004 M2005 K2006 E2011 I2012 D2013 G2014 N2022 I2027 N2031 T2032 E2033 D2034 G2035 F2036 H2042 N2043 E2044 D2045 L2046 G2047 N2048 E2049 E2050 G2051 E2052 E2053 I2054 S2055 Y2056 S2057 G2058 I2059 L2060 N2061 F2062 N2063 N2064 K2065 I2066 D2071
A2075 V2076 V2077 E2083 D2084 G2085 Y2089 E2092 D2093 T2094 A2095 E2096 L2101 S2102 L2103 I2104 N2105 D2106 G2107 D2113 D2114 F2121 V2122 T2123 I2124 N2125 D2126 K2127 Y2130 F2131 S2132 D2133 S2134 G2135 I2136 I2137 E2138 S2139 G2140 V2141 Q2142 N2143 I2144 D2145 D2146 N2147 Y2148 F2149 Y2150 I2151 D2152 D2153
N2154 G2155 I2156 V2157 Q2158 I2159 G2160 V2161 F2162 D2163 T2164 S2165 D2166 G2167 Y2168 K2169 Y2170 F2171 A2172 P2173 A2174 N2175 T2176 V2177 N2178 Y2182 A2185 V2186 E2187 Y2188 S2189 G2190 L2191 V2192 R2193 V2194 GLY GLU ASP VAL TYR TYR PHE GLY GLU THR TYR THR ILE GLU THR GLY TRP ILE TYR ASP MET GLU
ASN GLU SER ASP LYS TYR TYR PHE ASN PRO GLU THR LYS LYS ALA CYS LYS GLY ILE ASN LEU ILE ASP ASP ILE LYS TYR TYR PHE ASP GLU LYS GLY ILE MET ARG THR GLY LEU ILE SER PHE GLU ASN ASN ASN TYR TYR PHE ASN GLU ASN GLY GLU MET GLN PHE GLY TYR ILE



• Molecule 2: Frizzled-7

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151385	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.453	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.875	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	579.6, 579.6, 579.6	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1592, 1.1592, 1.1592	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/17497	0.46	0/23686
2	B	0.26	0/974	0.48	0/1325
All	All	0.29	0/18471	0.46	0/25011

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	17176	0	16623	207	0
2	B	949	0	910	15	0
3	A	1	0	0	0	0
All	All	18126	0	17533	221	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 6.

All (221) 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:907:GLU:N	1:A:907:GLU:OE1	2.14	0.80
1:A:299:GLU:O	1:A:300:SER:OG	2.02	0.76
1:A:40:ASN:ND2	1:A:44:GLU:OE1	2.20	0.74
1:A:876:ASN:ND2	1:A:912:GLU:OE1	2.20	0.73
1:A:669:ASP:OD1	1:A:718:LYS:NZ	2.22	0.73
1:A:837:VAL:O	1:A:840:ARG:NH1	2.22	0.73
1:A:1149:ASP:OD1	1:A:1228:ARG:NH2	2.24	0.71
1:A:1184:ILE:HD12	1:A:1185:ASP:N	2.08	0.68
2:B:125:GLU:OE1	2:B:128:ARG:NH2	2.26	0.68
1:A:1653:GLN:OE1	1:A:1689:ASN:ND2	2.25	0.68
2:B:67:LEU:HD12	2:B:107:ALA:O	1.93	0.68
1:A:74:LYS:NZ	1:A:867:ASP:OD1	2.26	0.67
1:A:587:ASP:OD2	1:A:653:HIS:NE2	2.26	0.67
1:A:1625:CYS:SG	1:A:1626:ASP:N	2.68	0.67
1:A:455:ARG:NE	1:A:823:GLU:OE2	2.29	0.66
1:A:872:LEU:HD11	1:A:911:VAL:HG12	1.77	0.66
1:A:748:SER:OG	1:A:749:GLU:OE1	2.13	0.64
1:A:1558:ASP:OD1	1:A:1559:GLU:N	2.29	0.64
1:A:1184:ILE:HD13	1:A:1266:TYR:CD1	2.33	0.63
1:A:1711:ASN:OD1	1:A:1711:ASN:N	2.32	0.62
2:B:78:ASP:OD1	2:B:79:ALA:N	2.31	0.62
1:A:1366:ASP:OD1	1:A:1367:LEU:N	2.32	0.62
1:A:1106:LEU:HD13	1:A:1107:VAL:H	1.65	0.62
1:A:385:GLN:NE2	1:A:515:GLU:OE2	2.32	0.61
1:A:1912:ASN:N	1:A:1917:ASN:O	2.28	0.61
1:A:1429:ILE:HD11	1:A:1447:ILE:HD11	1.83	0.61
1:A:1353:ARG:NH1	1:A:1407:SER:O	2.34	0.60
1:A:1433:LEU:N	1:A:1471:GLU:OE1	2.35	0.60
2:B:164:ASN:O	2:B:165:THR:OG1	2.19	0.59
1:A:1184:ILE:HD13	1:A:1266:TYR:CE1	2.36	0.59
1:A:1129:LEU:O	1:A:1133:GLU:N	2.35	0.59
1:A:87:LYS:NZ	1:A:88:ASN:OD1	2.36	0.59
1:A:1548:LYS:O	1:A:1603:LYS:N	2.34	0.59
1:A:283:MET:CB	1:A:388:ILE:HG22	2.33	0.59
1:A:339:ASP:OD1	1:A:340:GLU:N	2.35	0.59
1:A:6:ARG:NH1	1:A:29:ASP:OD1	2.36	0.58
1:A:1121:VAL:O	1:A:1125:LYS:N	2.26	0.57
1:A:1025:LEU:HD11	1:A:1035:ILE:HG23	1.86	0.57
1:A:873:LYS:NZ	1:A:879:GLU:O	2.38	0.57
1:A:598:PHE:HD1	1:A:605:SER:HG	1.51	0.57
1:A:855:ILE:HD11	1:A:1651:ASN:HD21	1.70	0.57
2:B:83:VAL:O	2:B:86:PHE:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:LEU:HD13	1:A:1203:TYR:HE2	1.69	0.56
2:B:83:VAL:HG13	2:B:106:TYR:CE2	2.40	0.56
2:B:111:THR:O	2:B:113:LEU:N	2.39	0.56
1:A:1984:VAL:O	1:A:1986:GLN:NE2	2.38	0.56
1:A:138:ILE:HG21	1:A:265:LEU:HD21	1.88	0.55
1:A:1498:TYR:O	1:A:1500:ASP:N	2.39	0.55
1:A:1625:CYS:HA	1:A:1631:ILE:HA	1.88	0.55
1:A:23:GLU:OE1	1:A:23:GLU:N	2.34	0.55
1:A:1766:ARG:NH2	1:A:1804:TYR:OH	2.40	0.55
1:A:884:ILE:HD12	1:A:884:ILE:H	1.72	0.54
2:B:50:GLN:O	2:B:65:THR:N	2.41	0.54
1:A:323:TYR:HB2	1:A:350:LEU:HD13	1.90	0.53
1:A:1252:ASP:OD1	1:A:1264:TRP:NE1	2.39	0.53
1:A:1100:SER:N	1:A:1148:ASP:OD2	2.42	0.52
1:A:1275:ILE:HD11	1:A:1278:LEU:HD21	1.90	0.52
1:A:120:ASP:OD2	1:A:356:LYS:NZ	2.36	0.52
1:A:1113:LEU:HD13	1:A:1120:VAL:HG13	1.92	0.52
1:A:2151:ILE:HD11	1:A:2155:GLY:HA2	1.92	0.52
1:A:893:ASP:OD1	1:A:894:GLU:N	2.43	0.52
1:A:1171:ARG:NH1	1:A:1197:GLU:O	2.43	0.52
1:A:784:GLU:OE1	1:A:784:GLU:N	2.43	0.51
1:A:2141:VAL:HG23	1:A:2143:ASN:O	2.09	0.51
1:A:959:LEU:HB2	1:A:1650:GLY:HA3	1.90	0.51
1:A:1749:PHE:HZ	1:A:1795:ILE:HG21	1.75	0.51
1:A:558:ASP:O	1:A:561:TYR:N	2.42	0.51
1:A:1164:LEU:HD12	1:A:1210:LYS:HE2	1.92	0.51
1:A:1291:LEU:HB2	1:A:1323:TYR:CZ	2.46	0.51
1:A:749:GLU:OE1	1:A:749:GLU:N	2.44	0.51
1:A:1552:LEU:HD23	1:A:1585:LEU:HD13	1.92	0.51
1:A:575:ARG:NE	1:A:601:THR:OG1	2.42	0.51
1:A:1483:LEU:HG	1:A:1527:LEU:HD21	1.93	0.51
1:A:1492:VAL:HG11	1:A:1516:VAL:HG21	1.93	0.50
1:A:835:GLN:O	1:A:839:GLU:N	2.44	0.50
1:A:1731:VAL:N	1:A:1781:SER:O	2.37	0.50
1:A:600:LYS:NZ	1:A:744:VAL:O	2.38	0.50
1:A:1483:LEU:HD21	1:A:1527:LEU:HG	1.94	0.50
1:A:1659:PRO:HD3	1:A:1674:ILE:HD11	1.93	0.50
1:A:1483:LEU:HD11	1:A:1527:LEU:HD11	1.93	0.50
1:A:1154:GLU:HB3	1:A:1163:VAL:HG12	1.92	0.50
1:A:173:ARG:NE	1:A:766:GLU:OE2	2.42	0.50
1:A:1184:ILE:HG12	1:A:1267:PHE:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2036:PHE:HB2	1:A:2075:ALA:HB3	1.94	0.50
1:A:1583:SER:HA	1:A:1631:ILE:HD11	1.94	0.49
1:A:883:PHE:HB2	1:A:901:ILE:HB	1.94	0.49
1:A:1881:ILE:HG22	1:A:1884:LYS:H	1.77	0.49
1:A:1624:ILE:HB	1:A:1634:TYR:HB2	1.95	0.49
1:A:375:ILE:HD13	1:A:382:ILE:HG23	1.94	0.49
1:A:653:HIS:O	1:A:664:ALA:N	2.43	0.49
1:A:1184:ILE:HG21	1:A:1265:ARG:O	2.12	0.49
1:A:1672:THR:O	1:A:1672:THR:OG1	2.29	0.49
1:A:1907:TYR:CE2	1:A:1909:ALA:HB2	2.47	0.49
1:A:778:ILE:HG23	1:A:787:ILE:HG23	1.94	0.49
1:A:1634:TYR:HA	1:A:1649:VAL:HG13	1.94	0.49
1:A:881:SER:HA	1:A:902:ASN:HA	1.95	0.48
1:A:1000:THR:HG22	1:A:1001:ILE:N	2.28	0.48
1:A:581:ILE:HD12	1:A:581:ILE:H	1.77	0.48
1:A:1113:LEU:HD13	1:A:1120:VAL:HG22	1.95	0.48
1:A:1336:ILE:HD11	1:A:1391:PHE:CE2	2.48	0.48
1:A:1634:TYR:HA	1:A:1649:VAL:CG1	2.43	0.48
1:A:612:ILE:O	1:A:615:SER:OG	2.25	0.48
1:A:1703:ASN:OD1	1:A:1732:ASN:ND2	2.39	0.48
1:A:154:LEU:HD11	1:A:534:TYR:HB3	1.95	0.48
1:A:1935:ILE:HB	1:A:1965:ALA:HB3	1.96	0.48
2:B:103:CYS:O	2:B:107:ALA:N	2.47	0.48
1:A:1901:THR:OG1	1:A:1902:GLU:N	2.46	0.48
1:A:1219:LEU:HD11	1:A:1299:ILE:HG12	1.96	0.47
1:A:461:ASP:OD1	1:A:463:LYS:NZ	2.47	0.47
1:A:21:GLU:OE1	1:A:21:GLU:N	2.39	0.47
1:A:608:PHE:CD2	1:A:618:ALA:HB2	2.49	0.47
1:A:1168:GLU:HG3	1:A:1201:SER:HA	1.95	0.47
1:A:989:VAL:HG13	1:A:993:LEU:HD12	1.95	0.47
1:A:1672:THR:OG1	1:A:1700:ASP:OD1	2.31	0.47
1:A:1349:ASP:OD2	1:A:1364:LYS:NZ	2.22	0.47
1:A:1970:ASN:OD1	1:A:1971:GLN:N	2.48	0.47
1:A:1375:LEU:HD23	1:A:1425:TYR:CG	2.50	0.47
1:A:1485:VAL:HG11	1:A:1516:VAL:HB	1.97	0.47
1:A:899:ARG:CZ	1:A:901:ILE:HD11	2.45	0.46
1:A:1357:ILE:HG12	1:A:1362:ILE:HG22	1.97	0.46
1:A:1120:VAL:HG21	1:A:1276:THR:O	2.15	0.46
1:A:1175:GLY:O	1:A:1261:GLU:N	2.43	0.46
1:A:1717:VAL:HB	1:A:1765:ILE:HG23	1.96	0.46
1:A:18:ARG:HG2	1:A:1667:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1355:VAL:HG13	1:A:1362:ILE:HB	1.97	0.46
1:A:2089:TYR:CG	1:A:2104:ILE:HD13	2.50	0.46
1:A:124:ASP:OD1	1:A:124:ASP:N	2.47	0.46
1:A:1598:LEU:HD11	2:B:139:GLY:HA3	1.98	0.46
1:A:224:TYR:O	1:A:228:SER:OG	2.29	0.45
1:A:1237:THR:N	1:A:1238:PRO:HD3	2.32	0.45
2:B:73:HIS:CG	2:B:79:ALA:HB2	2.51	0.45
1:A:1144:MET:HE1	1:A:1214:ASP:O	2.16	0.45
1:A:1151:VAL:HG11	1:A:1227:ASN:HA	1.98	0.45
1:A:1565:ILE:HD12	1:A:1612:ILE:CD1	2.47	0.45
1:A:283:MET:CG	1:A:388:ILE:HG22	2.47	0.45
1:A:1222:LEU:HD21	1:A:1298:PHE:HE2	1.82	0.45
1:A:1349:ASP:OD1	1:A:1407:SER:N	2.48	0.45
1:A:1498:TYR:HH	1:A:1506:PHE:HE2	1.65	0.45
1:A:1548:LYS:HB2	1:A:1602:ILE:HA	1.98	0.45
1:A:283:MET:HB2	1:A:388:ILE:HG22	1.98	0.44
1:A:557:VAL:HG23	1:A:609:GLN:OE1	2.17	0.44
1:A:1437:MET:HG2	1:A:1497:VAL:HG11	1.98	0.44
2:B:83:VAL:HG13	2:B:106:TYR:HE2	1.81	0.44
1:A:1185:ASP:OD1	1:A:1186:HIS:N	2.41	0.44
1:A:696:LEU:HD12	1:A:740:ASN:HB2	2.00	0.44
1:A:1958:PHE:HA	1:A:1965:ALA:HA	2.00	0.44
1:A:855:ILE:HD11	1:A:1651:ASN:ND2	2.30	0.44
1:A:711:TYR:HB3	1:A:712:PRO:HD3	2.00	0.44
1:A:1025:LEU:HD12	1:A:1033:ALA:HB1	1.99	0.44
1:A:1699:THR:O	1:A:1729:ILE:HD12	2.18	0.44
1:A:1878:GLU:OE2	1:A:1901:THR:OG1	2.27	0.44
1:A:1880:ILE:HG22	1:A:1882:ASP:H	1.83	0.44
1:A:270:ASP:O	1:A:273:ARG:HG2	2.18	0.44
1:A:446:PHE:CZ	1:A:450:LEU:HD11	2.52	0.44
1:A:546:ASP:N	1:A:546:ASP:OD1	2.50	0.44
1:A:134:ASN:O	1:A:203:ASP:N	2.51	0.43
1:A:456:VAL:HG11	1:A:465:THR:HG23	2.00	0.43
1:A:1360:ASP:OD1	1:A:1361:LYS:N	2.48	0.43
1:A:1677:SER:HA	1:A:1705:THR:HB	2.00	0.43
1:A:1412:ILE:HD13	1:A:1443:ILE:HD11	1.99	0.43
1:A:904:GLU:OE1	1:A:904:GLU:N	2.52	0.43
1:A:703:TYR:CD1	1:A:710:THR:HG21	2.53	0.43
1:A:1346:ILE:O	1:A:1404:LEU:HA	2.18	0.43
1:A:573:SER:OG	1:A:575:ARG:NE	2.51	0.43
1:A:1094:VAL:O	1:A:1096:LEU:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:ASP:OD1	1:A:1446:LYS:NZ	2.52	0.43
1:A:580:TYR:CZ	1:A:608:PHE:HZ	2.37	0.43
1:A:932:ILE:O	1:A:935:THR:OG1	2.32	0.43
1:A:1636:ILE:HG23	1:A:1638:PHE:CE1	2.54	0.43
1:A:137:LEU:O	1:A:206:VAL:HG11	2.18	0.43
1:A:1622:GLU:O	1:A:1634:TYR:N	2.52	0.43
1:A:1195:TYR:O	1:A:1196:ARG:NH1	2.38	0.43
1:A:1412:ILE:CD1	1:A:1443:ILE:HD11	2.48	0.43
2:B:142:TRP:O	2:B:143:PRO:C	2.57	0.43
1:A:1689:ASN:OD1	1:A:1690:LYS:N	2.52	0.43
1:A:1846:LYS:O	1:A:1850:ASN:N	2.50	0.42
1:A:2048:ASN:HB2	1:A:2052:GLU:HG2	2.00	0.42
1:A:432:ILE:HA	1:A:435:ILE:HG12	2.01	0.42
1:A:495:GLU:O	1:A:499:ARG:HG2	2.20	0.42
1:A:754:LEU:HD12	1:A:754:LEU:O	2.20	0.42
1:A:1160:ASN:HA	1:A:1215:LEU:HD12	2.00	0.42
1:A:1649:VAL:HG23	1:A:1650:GLY:N	2.34	0.42
1:A:117:GLN:NE2	1:A:326:TYR:HB3	2.34	0.42
1:A:118:TRP:CE2	1:A:285:LEU:HD13	2.54	0.42
1:A:1180:VAL:HG12	1:A:1181:THR:HG23	2.01	0.42
1:A:872:LEU:CD2	1:A:898:ILE:HG21	2.49	0.42
1:A:2142:GLN:NE2	1:A:2149:PHE:O	2.49	0.42
1:A:202:ILE:O	1:A:206:VAL:HG23	2.20	0.42
1:A:635:LYS:NZ	1:A:684:GLU:OE1	2.52	0.42
1:A:307:VAL:HG13	1:A:311:PHE:HD2	1.83	0.42
1:A:902:ASN:OD1	1:A:903:LYS:N	2.50	0.42
1:A:1025:LEU:HB3	1:A:1026:SER:H	1.76	0.42
1:A:1164:LEU:HD13	1:A:1203:TYR:CE2	2.53	0.42
1:A:1181:THR:OG1	1:A:1185:ASP:OD2	2.37	0.42
1:A:1578:SER:O	1:A:1579:ASP:HB2	2.19	0.42
1:A:559:LYS:HB2	1:A:628:ILE:HB	2.01	0.42
1:A:1996:LYS:NZ	1:A:2049:GLU:OE1	2.53	0.42
2:B:74:THR:OG1	2:B:75:ASN:N	2.53	0.42
1:A:2060:LEU:O	1:A:2066:ILE:HA	2.20	0.41
1:A:835:GLN:NE2	1:A:838:GLU:OE1	2.53	0.41
1:A:1184:ILE:HD12	1:A:1184:ILE:C	2.40	0.41
1:A:1251:LEU:HA	1:A:1254:ILE:HD12	2.03	0.41
1:A:872:LEU:HD13	1:A:914:GLU:HG3	2.02	0.41
1:A:1323:TYR:O	1:A:1324:ALA:HB3	2.21	0.41
2:B:87:TYR:N	2:B:88:PRO:HD2	2.35	0.41
1:A:131:TYR:CD1	1:A:232:ILE:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:MET:HA	1:A:388:ILE:HG22	2.03	0.41
1:A:1291:LEU:HD21	1:A:1298:PHE:HE1	1.84	0.41
1:A:1287:ILE:HG22	1:A:1289:ILE:HG13	2.03	0.41
1:A:1329:GLN:NE2	1:A:1357:ILE:HD11	2.35	0.41
1:A:1621:PHE:CZ	1:A:1638:PHE:CE1	3.09	0.41
1:A:2045:ASP:OD1	1:A:2045:ASP:N	2.53	0.41
1:A:888:ASP:OD2	1:A:899:ARG:NH1	2.53	0.41
1:A:1289:ILE:HG22	1:A:1291:LEU:CD1	2.50	0.41
1:A:1721:ASP:OD1	1:A:1721:ASP:N	2.51	0.41
1:A:1584:PHE:O	1:A:1584:PHE:CG	2.74	0.40
1:A:334:HIS:NE2	1:A:709:GLU:OE2	2.46	0.40
1:A:1287:ILE:HD12	1:A:1287:ILE:N	2.37	0.40
1:A:1428:LEU:HG	1:A:1461:PRO:HG2	2.03	0.40
1:A:402:GLN:NE2	1:A:480:ASP:OD2	2.55	0.40
1:A:890:SER:O	1:A:896:PHE: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	2136/2397 (89%)	1959 (92%)	174 (8%)	3 (0%)	51 82
2	B	119/603 (20%)	99 (83%)	20 (17%)	0	100 100
All	All	2255/3000 (75%)	2058 (91%)	194 (9%)	3 (0%)	54 82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1499	MET
1	A	1631	ILE
1	A	1193	ILE

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	1930/2163 (89%)	1876 (97%)	54 (3%)	43 69
2	B	106/505 (21%)	104 (98%)	2 (2%)	57 76
All	All	2036/2668 (76%)	1980 (97%)	56 (3%)	46 69

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	124	ASP
1	A	228	SER
1	A	243	PHE
1	A	274	ILE
1	A	392	ASP
1	A	393	SER
1	A	508	ILE
1	A	510	GLN
1	A	522	PHE
1	A	543	LEU
1	A	571	ARG
1	A	575	ARG
1	A	580	TYR
1	A	983	VAL
1	A	994	PHE
1	A	998	LEU
1	A	1007	VAL
1	A	1025	LEU
1	A	1032	ILE
1	A	1035	ILE
1	A	1055	LEU
1	A	1057	ARG
1	A	1058	GLN
1	A	1067	MET
1	A	1076	THR
1	A	1106	LEU

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Mol	Chain	Res	Type
1	A	1116	LYS
1	A	1137	THR
1	A	1138	LEU
1	A	1163	VAL
1	A	1184	ILE
1	A	1194	THR
1	A	1232	TRP
1	A	1336	ILE
1	A	1387	HIS
1	A	1462	TYR
1	A	1476	ASN
1	A	1490	ASP
1	A	1494	ILE
1	A	1625	CYS
1	A	1661	TYR
1	A	1672	THR
1	A	1687	CYS
1	A	1711	ASN
1	A	1765	ILE
1	A	1770	VAL
1	A	1835	LEU
1	A	1856	PHE
1	A	1864	TYR
1	A	1884	LYS
1	A	1917	ASN
1	A	1972	ILE
1	A	2056	TYR
2	B	129	GLN
2	B	160	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	553	GLN
1	A	611	ASN
1	A	699	ASN
1	A	809	ASN
1	A	835	GLN
1	A	924	HIS
1	A	1070	ASN
1	A	1159	ASN

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Mol	Chain	Res	Type
1	A	1227	ASN
1	A	2147	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - 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.

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.

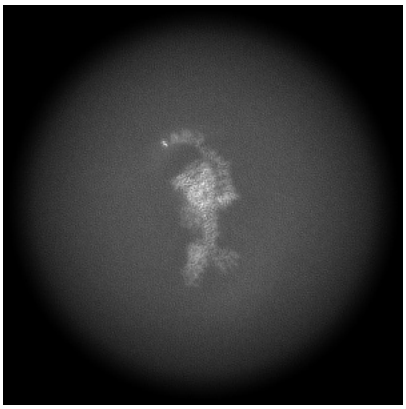
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18374. These allow visual inspection of the internal detail of the map and identification of artifacts.

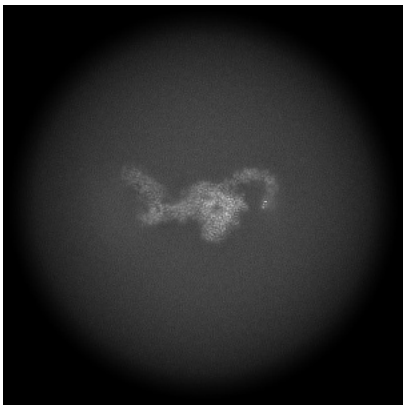
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

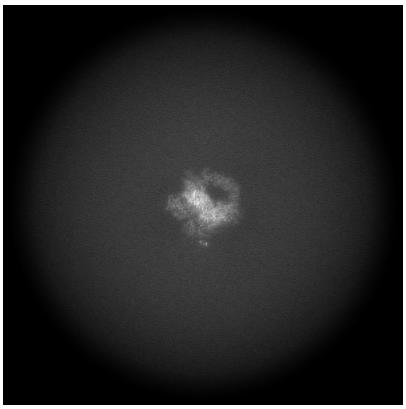
6.1.1 Primary map



X

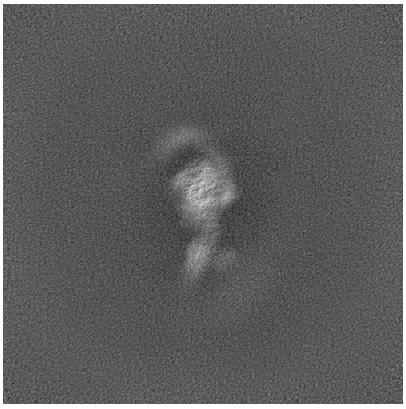


Y

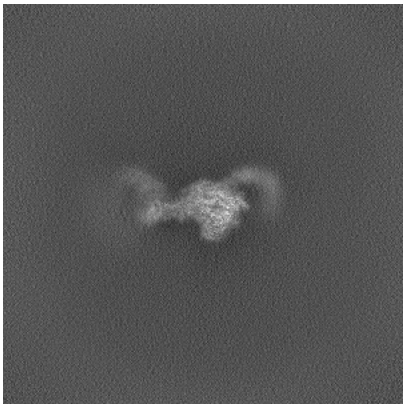


Z

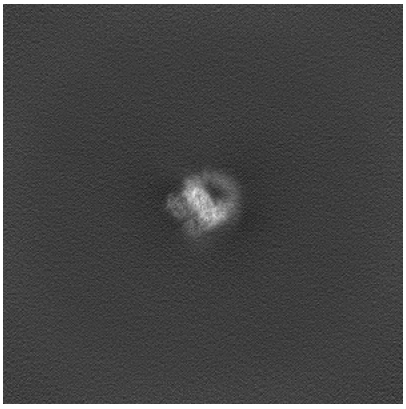
6.1.2 Raw map



X



Y

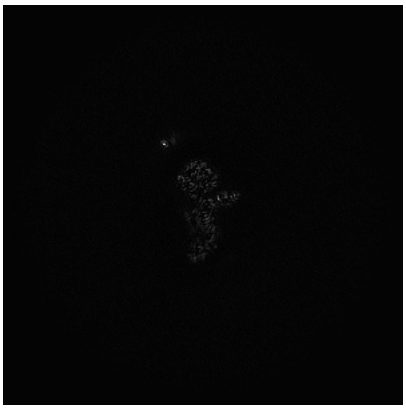


Z

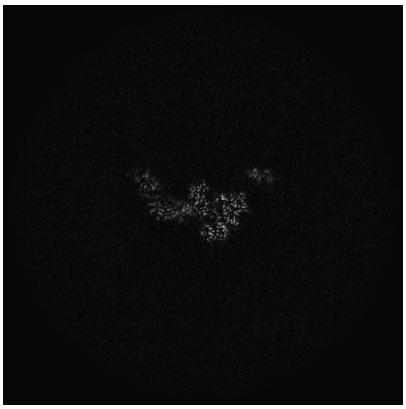
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

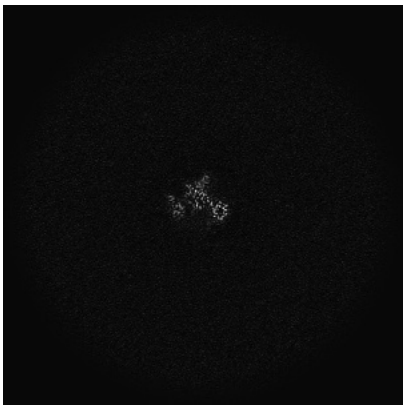
6.2.1 Primary map



X Index: 250

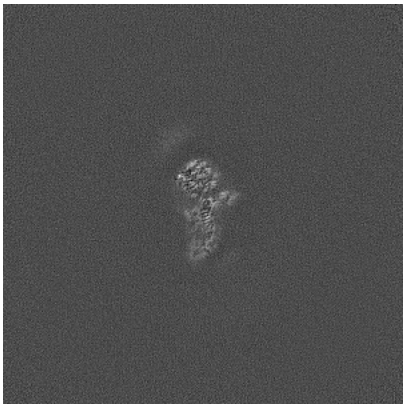


Y Index: 250

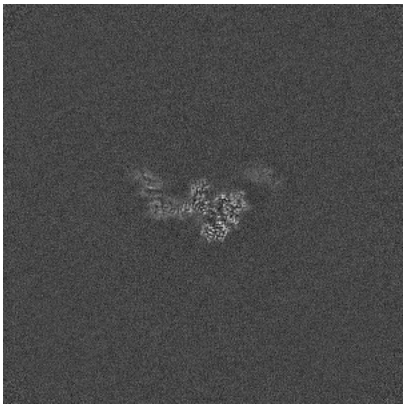


Z Index: 250

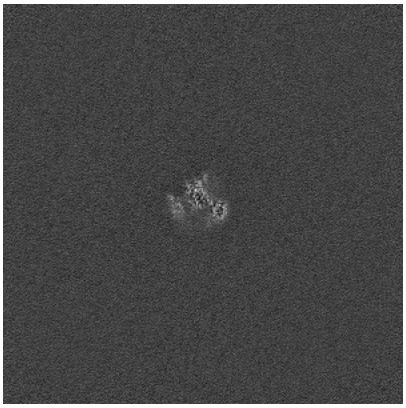
6.2.2 Raw map



X Index: 250



Y Index: 250

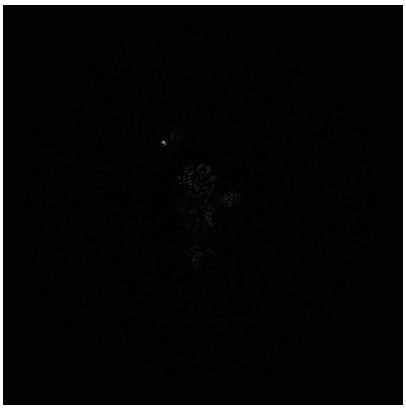


Z Index: 250

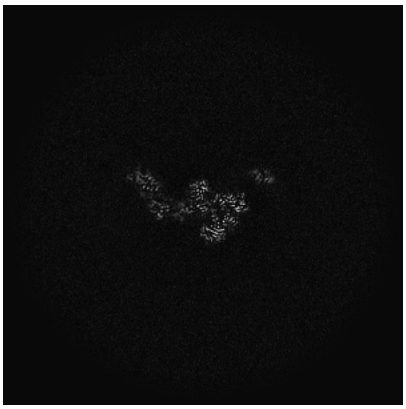
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

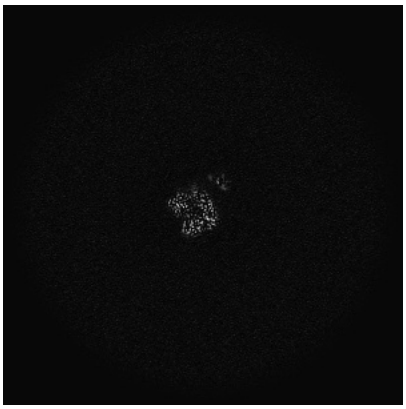
6.3.1 Primary map



X Index: 254

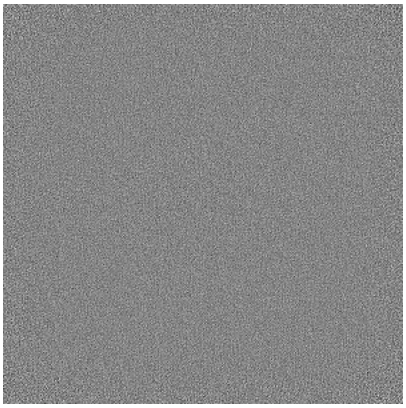


Y Index: 248

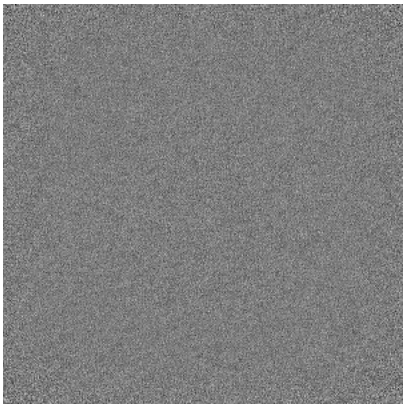


Z Index: 275

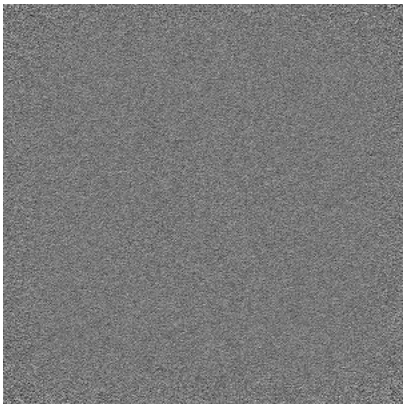
6.3.2 Raw map



X Index: 0



Y Index: 0

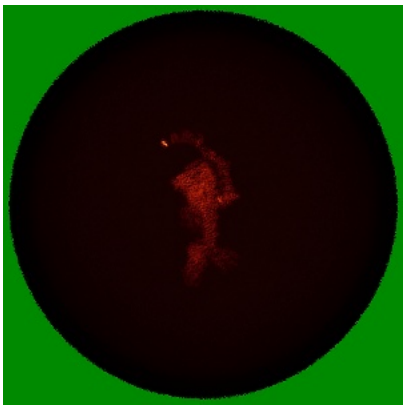


Z Index: 0

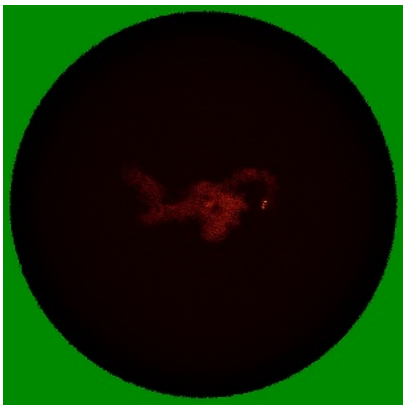
The images above show the largest variance slices of the map in three orthogonal directions.

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

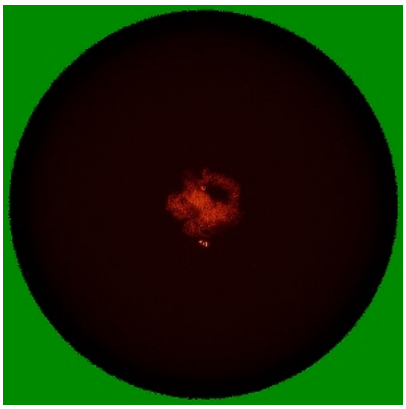
6.4.1 Primary map



X

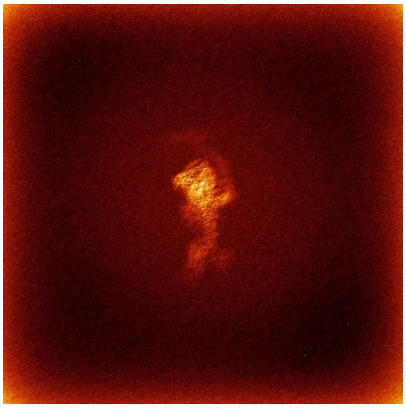


Y

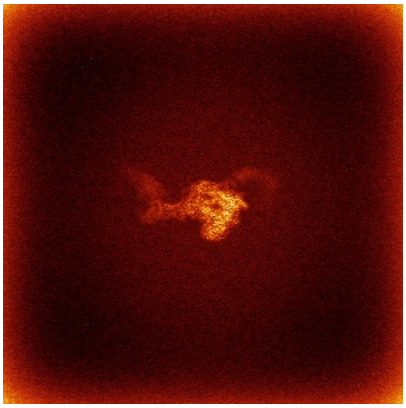


Z

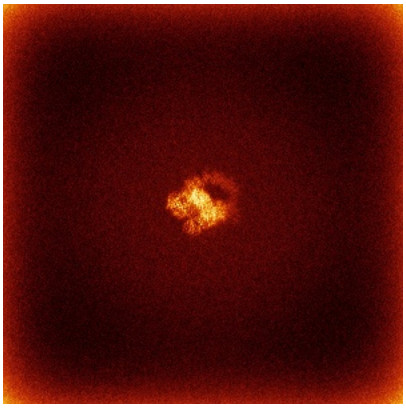
6.4.2 Raw map



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 0.4. 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.

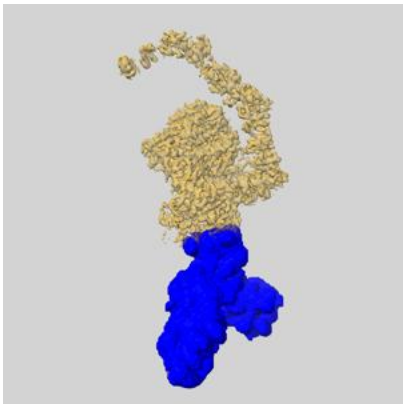
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

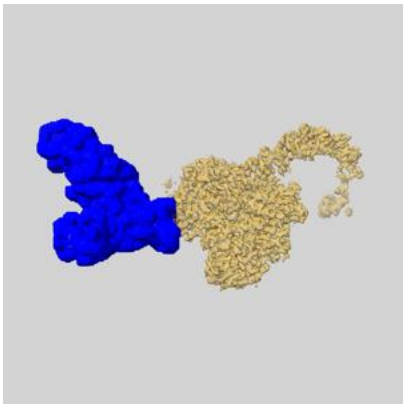
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

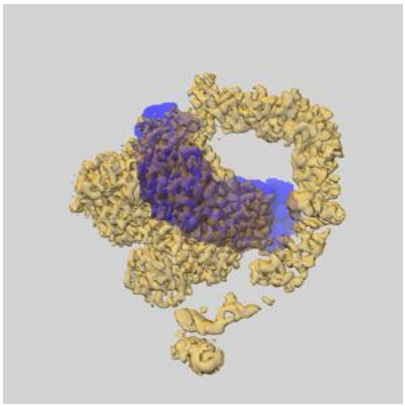
6.6.1 emd_18374_msk_1.map



X

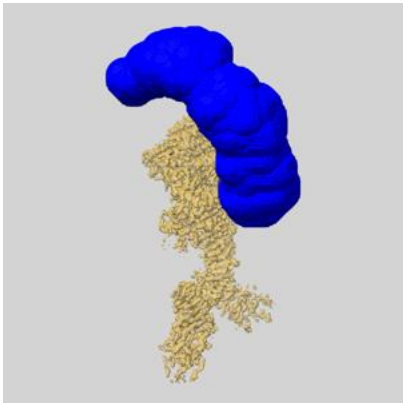


Y

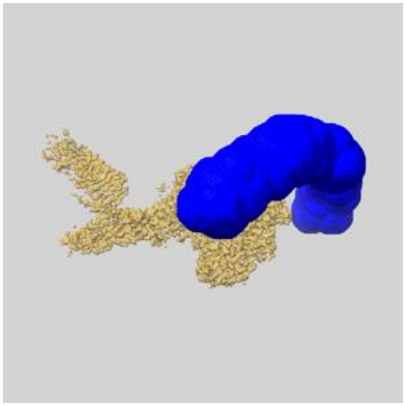


Z

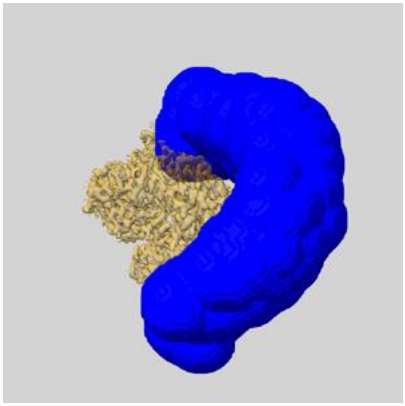
6.6.2 emd_18374_msk_2.map



X

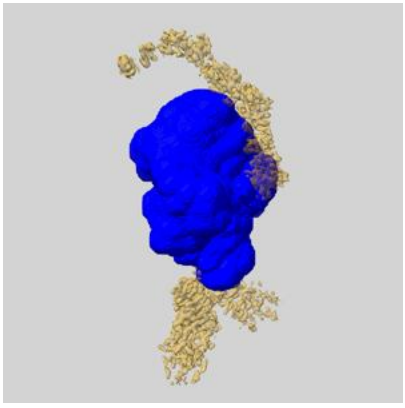


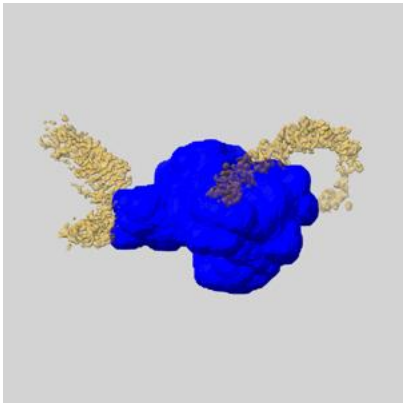
Y

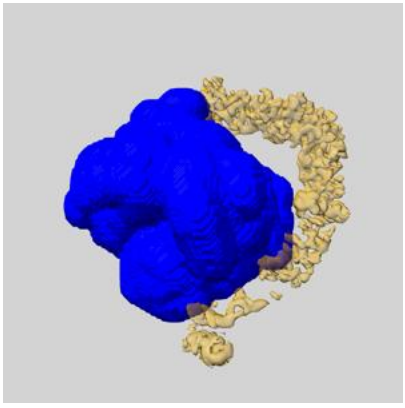


Z

6.6.3 emd_18374_msk_3.map


X

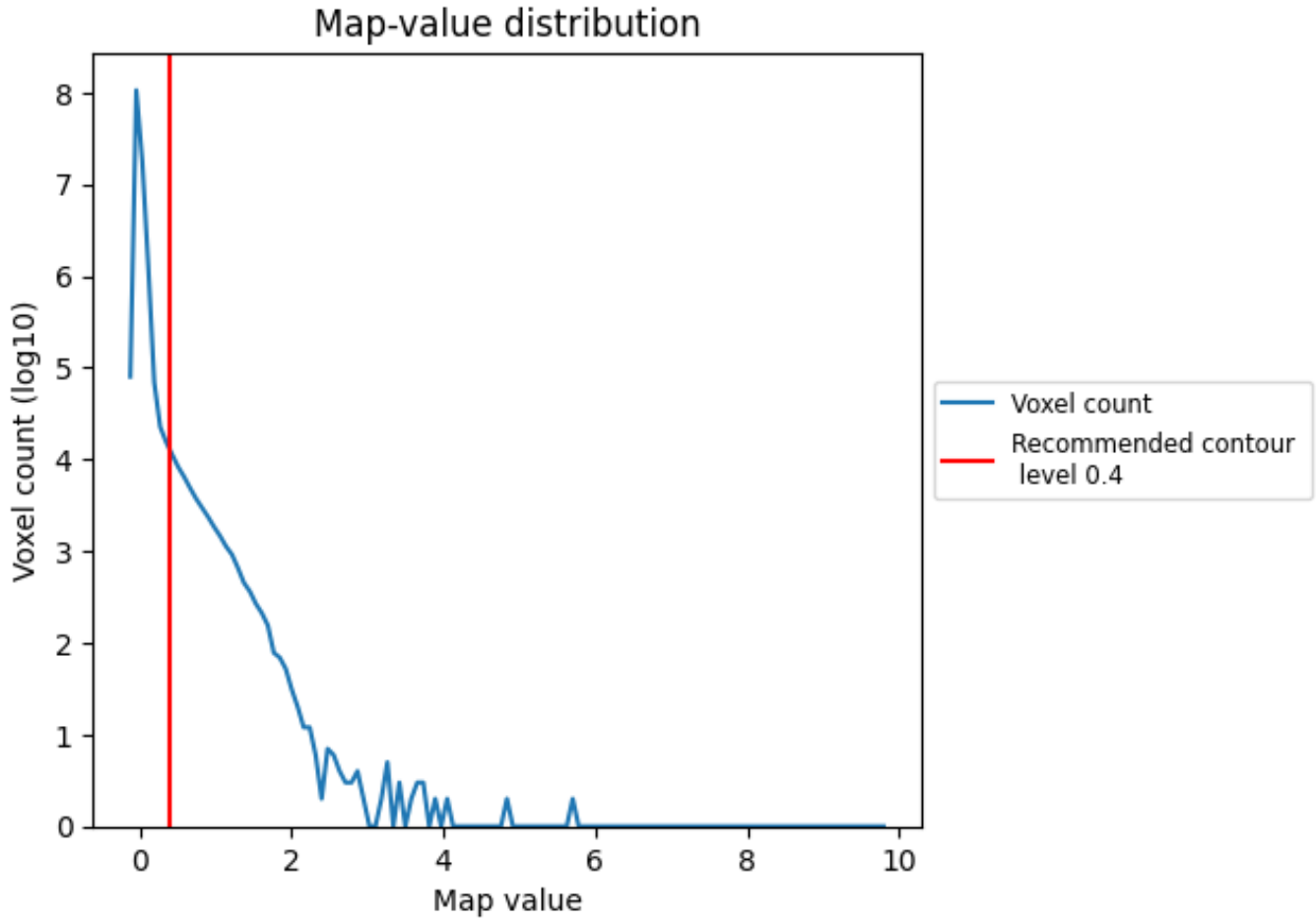

Y


Z

7 Map analysis

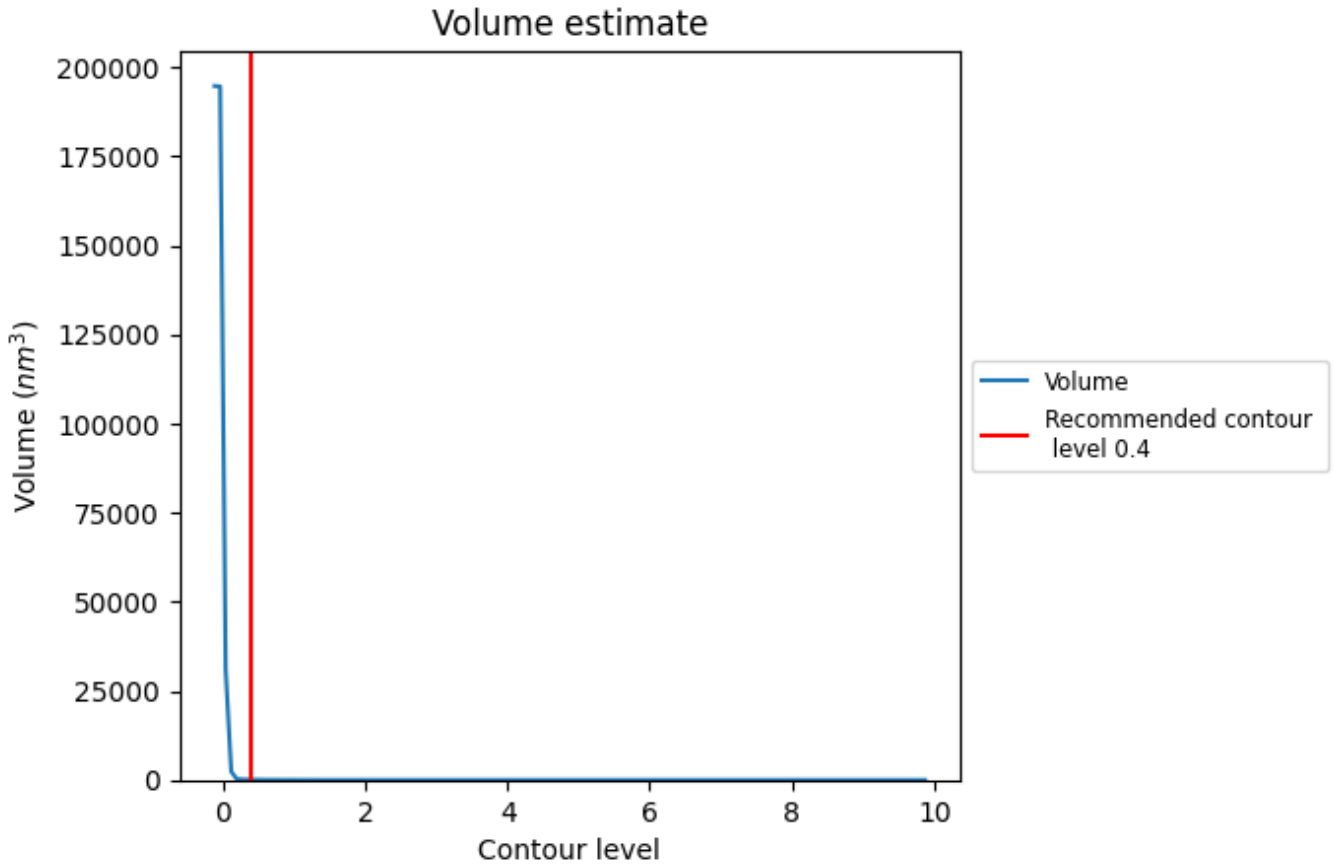
This section contains the results of statistical analysis of the map.

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.

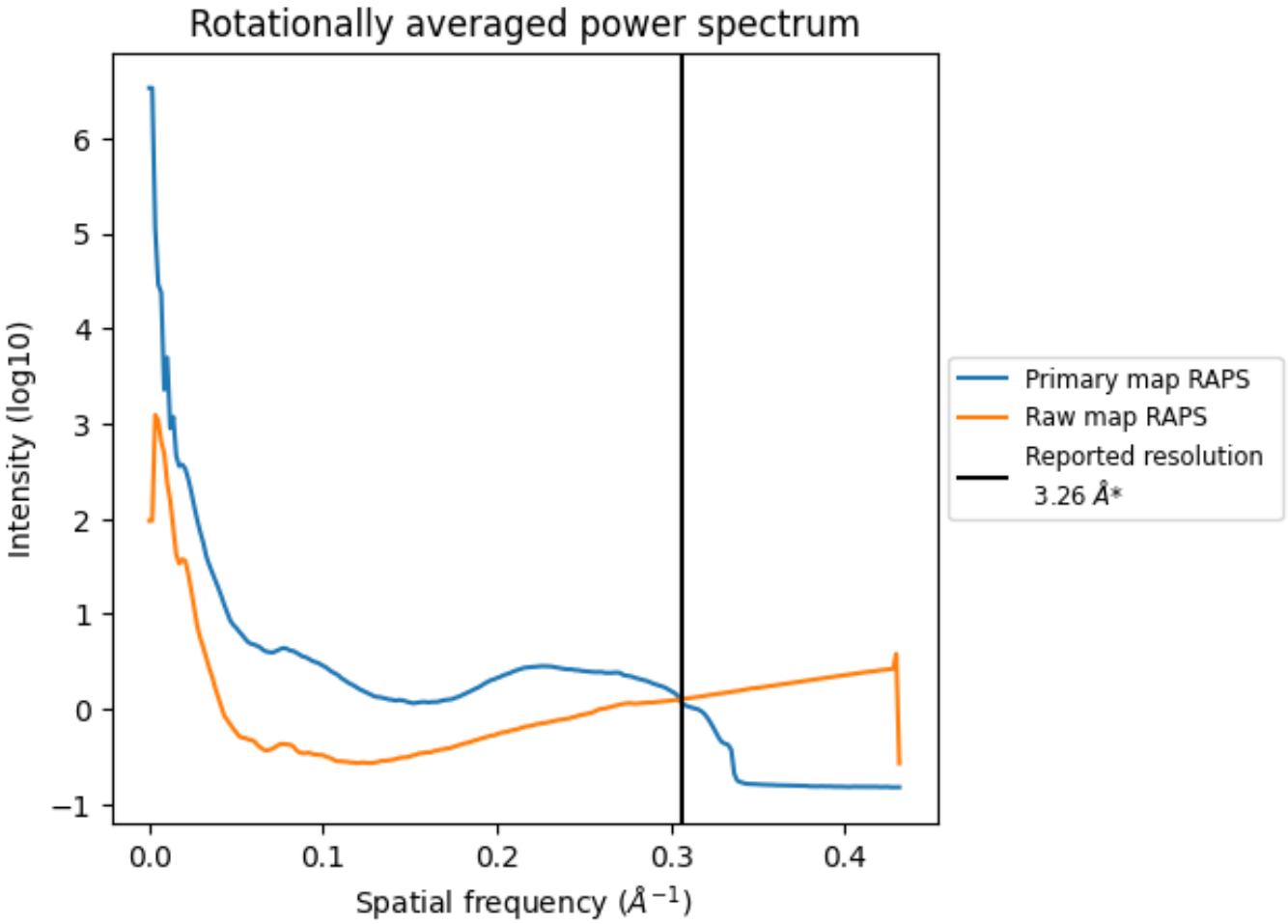
7.2 Volume estimate



The volume at the recommended contour level is 84 nm^3; this corresponds to an approximate mass of 75 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)

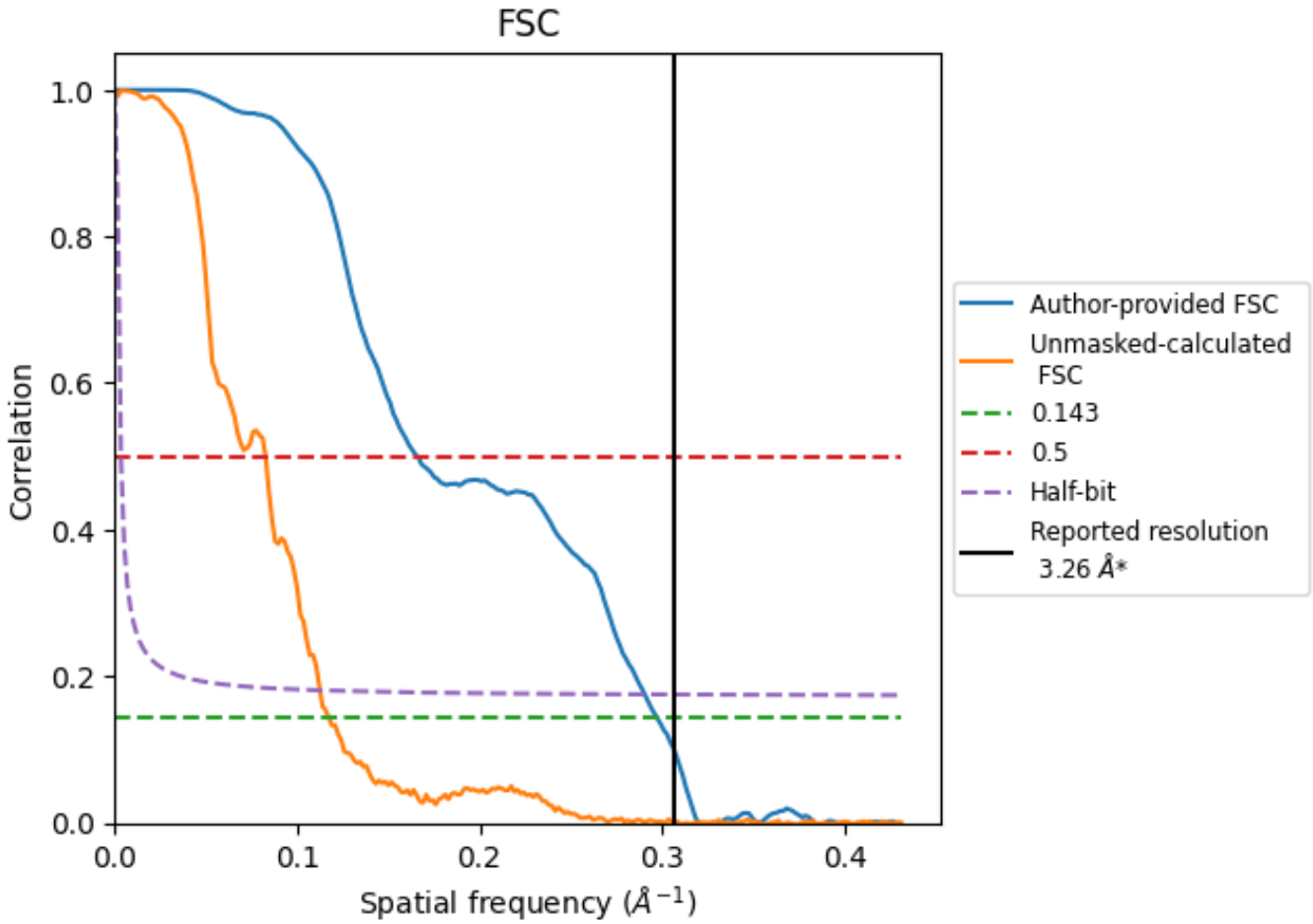


*Reported resolution corresponds to spatial frequency of 0.307 $Å^{-1}$

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 0.307 Å^{-1}

8.2 Resolution estimates (i)

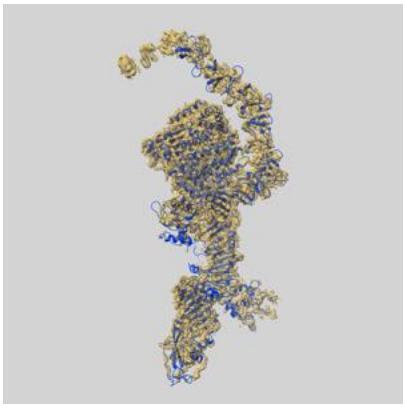
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.36	6.03	3.44
Unmasked-calculated*	8.51	12.09	8.88

*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 8.51 differs from the reported value 3.26 by more than 10 %

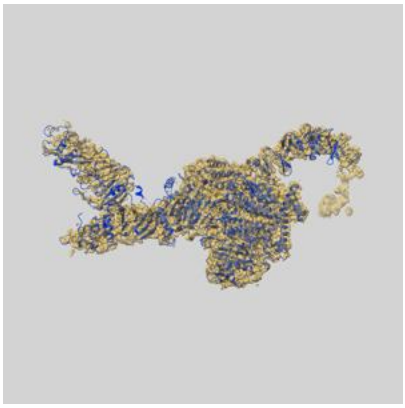
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18374 and PDB model 8QEO. Per-residue inclusion information can be found in section 3 on page 6.

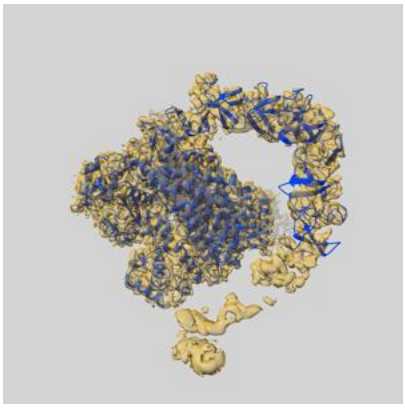
9.1 Map-model overlay



X



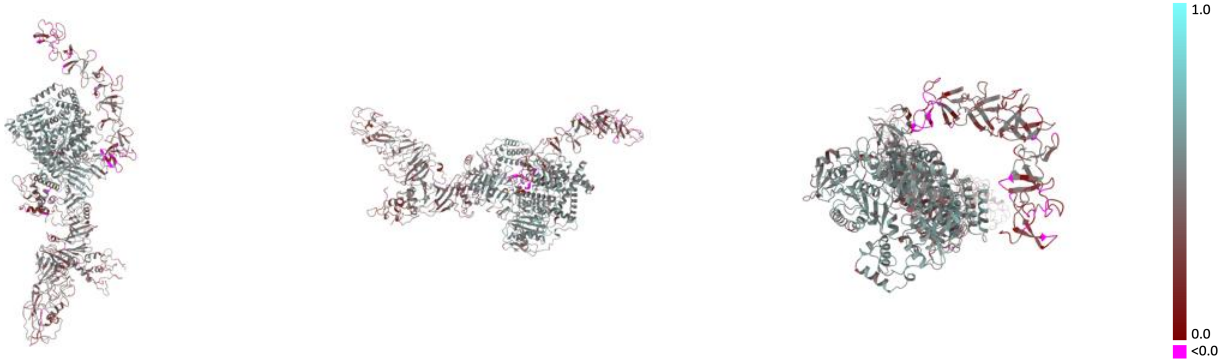
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

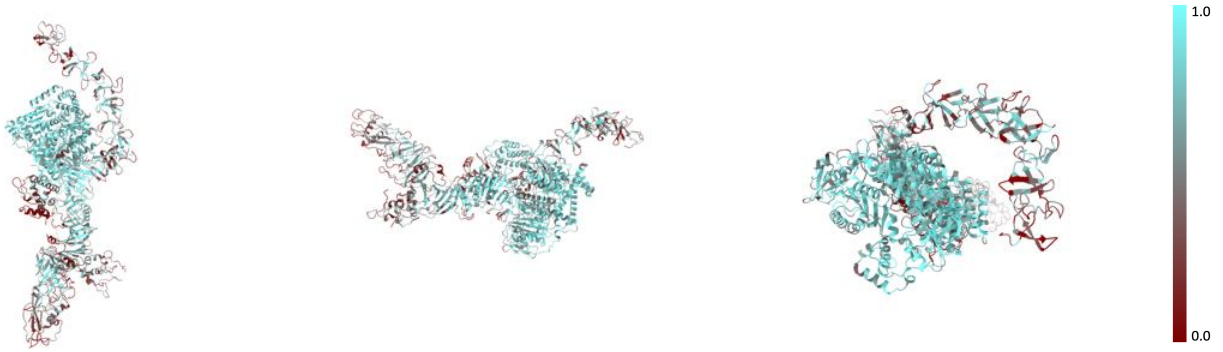
9.2 Q-score mapped to coordinate model (i)



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.

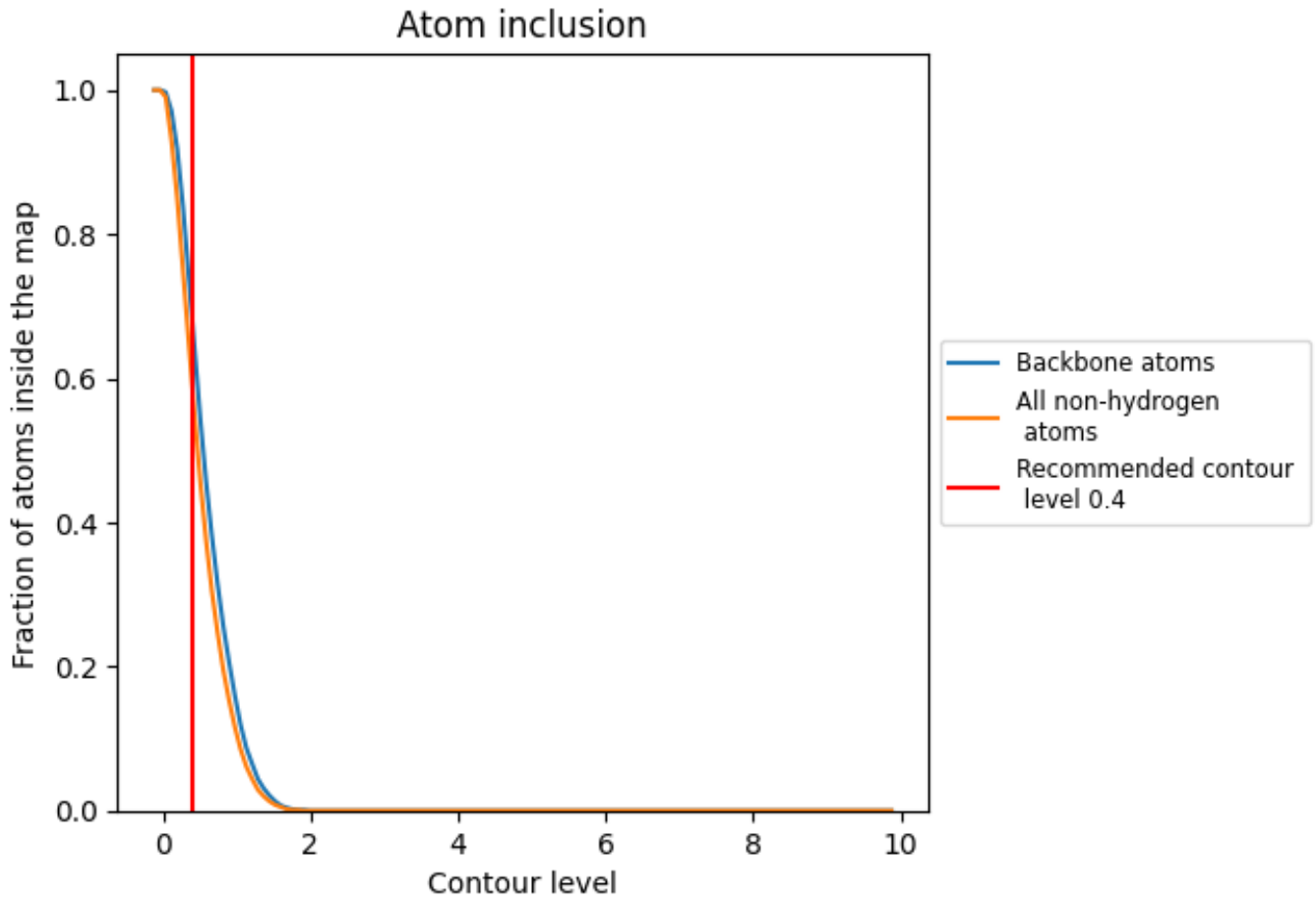
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 58% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5810	0.4160
A	0.5920	0.4200
B	0.3760	0.3350