



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:19 PM UTC

PDB ID : 8QEN / pdb_00008qen
EMDB ID : EMD-18373
Title : cryo-EM structure of apo Clostridioides difficile toxin B
Authors : Kinsolving, J.; Bous, J.; Structural Genomics Consortium (SGC)
Deposited on : 2023-09-01
Resolution : 3.40 Å(reported)
Based on initial model : .

This is a wwPDB EM Validation Summary 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

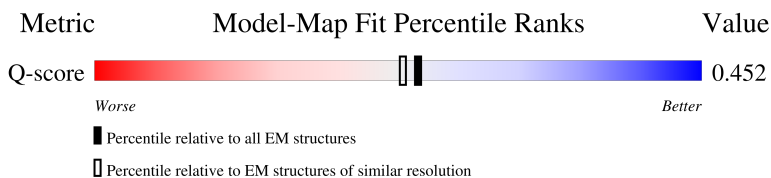
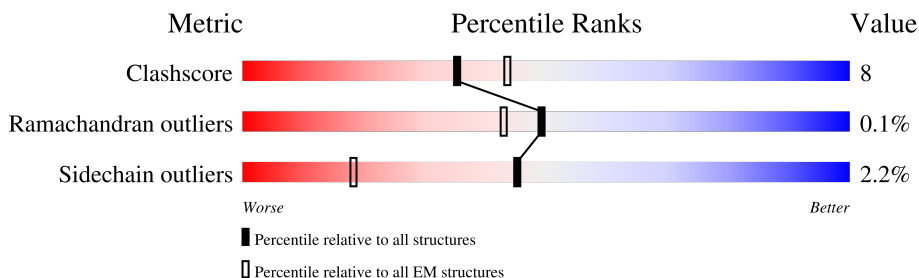
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 $\leq 5\%$. 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	34% 77% 20% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19007 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
1	A	2363	Total	C	N	O	S	0	0
			19006	12122	2981	3850	53		

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

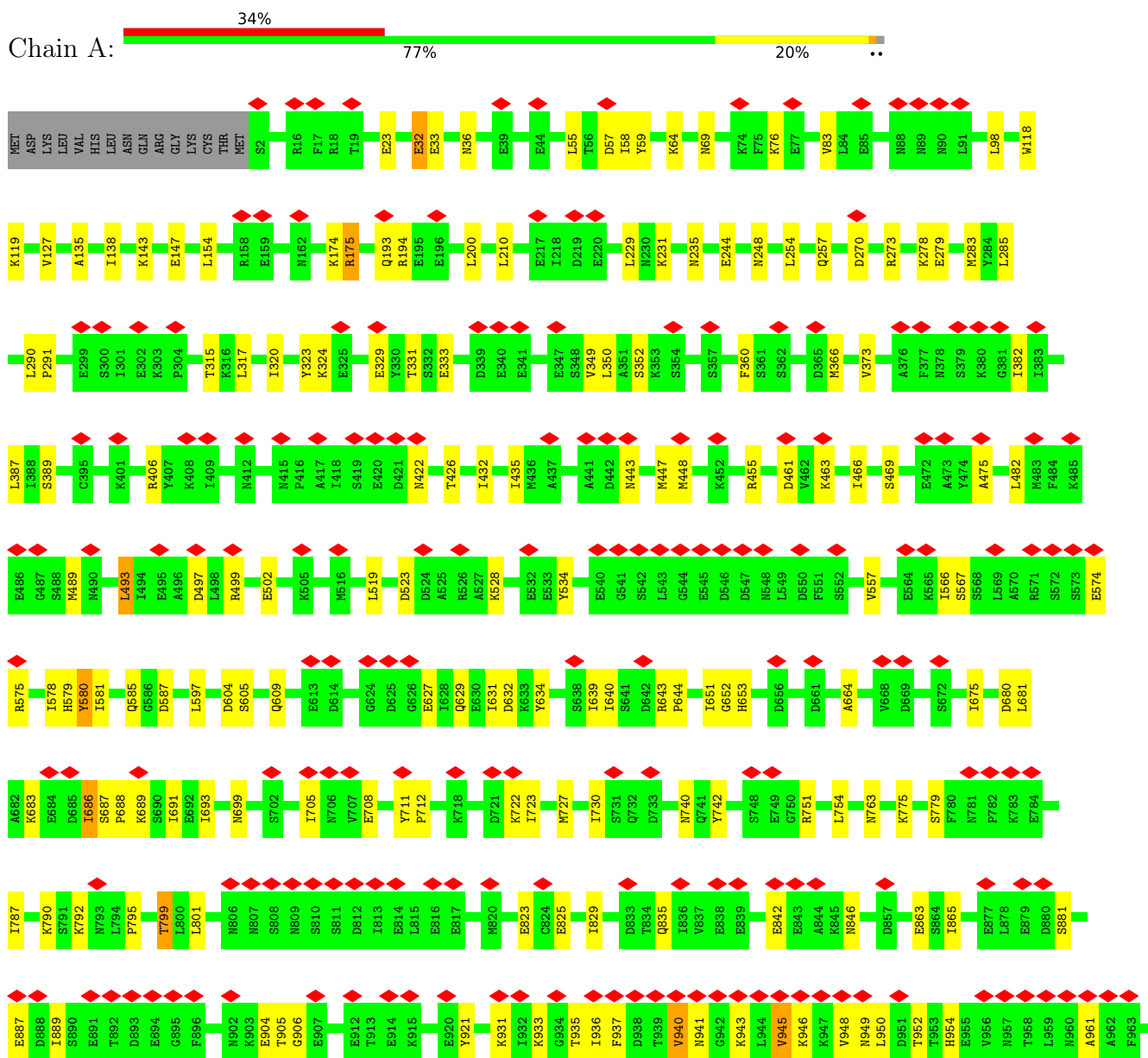
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

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



L968	S974	M985	K986	Q988	A991	Q992	T996	G997	I1001	T1002	D1003	A1004	A1005	K1006	E1009	L1010	D1016	E1017	T1018	I1019	D1020	L1021	L1022	P1023	T1024	L1025	S1026	E1027	G1028	L1029	P1030	I1031	I1032	A1033	T1034	I1035	I1036	D1037	G1038	V1039	S1040	L1041	G1042	A1043	A1044	I1045	K1046	E1047	E1050	T1051							
S1052	D1053	P1054	L1055	L1056	Q1057	E1058	I1060	E1061	A1062	K1063	I1064	G1065	I1066	T1067	E1076	A1077	S1080	S1081	S1082	G1083	I1085	A1086	S1087	G1088	F1089	S1090	I1091	L1092	L1093	L1096	A1097	G1098	I1099	S1100	P1104	V1107	L1108	N1109	E1110	L1111	V1112	L1113	R1114	D1115	K1116	A1117	T1118										
K1119	Y1123	F1124	K1125	H1126	V1127	E1131	T1132	E1133	L1138	L1139	D1140	D1141	K1142	D1148	D1149	E1154	M1159	N1160	L1164	I1169	M1172	E1173	S1176	T1179	V1180	T1181	D1182	D1183	I1184	D1185	H1186	F1187	S1188	S1189	A1190	P1191	R1196	E1197	D1204	V1205	L1206	L1207	V1208	Q1209	K1210	E1211											
E1212	L1213	D1214	L1215	S1216	K1217	D1218	L1219	P1223	N1224	A1225	P1226	F1230	A1231	W1232	E1233	T1234	G1235	W1236	T1237	P1238	G1239	R1241	S1242	L1243	E1244	N1245	D1246	G1247	T1248	K1249	L1250	L1251	I1254	R1255	D1256	E1261	W1264	R1265	Y1266	F1269	I1270	A1271	A1272	A1273	L1274	I1275	L1278	K1279	P1280	R1281	Y1282						
E1283	D1284	I1287	R1288	D1292	S1293	R1296	I1299	I1302	T1305	E1306	E1307	I1308	R1309	Y1314	T1322	S1326	L1327	Y1330	M1331	M1332	E1340	S1341	D1342	V1343	D1347	V1351	V1352	R1353	D1354	V1355	T1356	I1357	E1358	S1359	D1360	K1361	I1362	K1363	K1364	G1365	L1366	L1367	I1368	E1369	G1370	I1371											
L1372	S1373	T1374	L1375	S1376	I1377	E1378	E1379	N1380	N1385	S1386	H1387	I1388	I1389	E1394	F1401	S1407	I1408	L1409	E1410	G1411	I1412	N1413	V1418	D1419	L1420	L1421	L1428	G1431	E1432	M1437	L1438	N1439	S1440	N1441	H1442	I1443	Q1444	Q1445	T1447	D1448	Y1449	F1452	N1453	L1454	E1455	L1456	P1461	Y1462									
D1466	S1467	E1468	G1469	G1477	K1480	V1485	S1486	E1487	L1488	P1489	D1490	L1493	I1494	M1499	D1500	D1501	S1502	K1503	Y1508	Y1509	S1510	N1511	D1515	V1516	K1517	K1521	D1522	N1523	K1533	D1534	D1535	I1536	S1539	T1543	L1544	Q1545	D1546	E1547	L1548	T1549	I1550	V1555	H1556	L1557	D1558	E1559											
S1560	G1561	E1564	I1565	F1568	R1571	K1572	G1573	N1574	T1575	E1576	T1577	S1578	D1579	F1584	M1588	K1591	S1592	I1593	F1594	V1595	N1596	F1597	L1598	Q1599	S1600	N1601	I1602	K1603	D1607	A1608	I1612	S1617	I1618	F1621	I1624	E1627	N1628	P1633	Y1634	F1635	L1636	K1637	N1638	T1640	L1641												
E1642	T1643	N1644	Y1645	Y1648	R1652	I1656	V1657	E1658	P1659	N1660	Y1661	D1662	D1665	D1668	N1675	F1676	S1677	Q1678	K1679	Y1680	L1681	Y1682	G1683	I1684	D1685	S1686	C1687	K1690	V1691	V1692	I1693	S1694	D1700	Y1708	E1709	T1710	N1711	N1712	T1713	Y1714	P1715	E1716	D1721	A1722	E1727	I1738	R1739										
Y1740	V1741	D1745	D1748	F1749	S1753	T1754	S1755	E1756	E1757	M1758	K1759	V1760	S1761	Q1762	V1763	K1764	I1765	A1766	D1773	K1774	T1775	L1776	I1777	E1778	K1779	M1783	D1786	A1787	Y1788	D1789	V1790	E1794	I1795	T1800	Y1803	Y1804	E1805	D1806	G1807	L1808	I1809	G1810	Y1811	D1812	L1813	G1814	L1815	V1816	S1817	L1818							
Y1819	N1820	E1821	K1822	F1823	Y1824	I1825	N1826	N1827	F1828	R1829	M1830	S1833	G1834	L1835	I1836	Y1837	I1838	N1839	D1840	S1841	L1842	K1846	P1847	P1848	I1849	N1850	T1854	G1855	F1856	V1857	T1858	S1859	G1860	D1861	D1862	K1863	Y1864	Y1865	F1866	I1869	N1870	E1871	G1872	E1878	T1879	I1880	I1881	D1882	D1883	K1884	N1885	V1893	L1894				
Q1895	T1896	G1897	V1898	F1899	S1900	T1901	E1902	D1903	G1904	F1905	N1912	T1913	L1914	D1915	E1916	N1917	L1918	E1919	G1920	E1921	A1922	I1923	D1924	F1925	T1926	G1927	K1928	L1929	I1930	D2000	D1931	D1932	E1933	F1938	D1939	D1940	N1941	Y1942	G1943	G1944	A1945	V1946	E1947	W1948	K1949	E1950	L1951	D1952	G1953	E1954	M1955	H1956	E1961	T1962	G1963	K1964	A1965
F1966	K1967	G1968	L1969	N1970	Q1971	I1972	G1973	D1974	Y1975	K1976	N1980	S1981	D1982	K1987	G1988	F1989	V1990	S1991	I1992	N1993	D1994	N1995	K1996	H1997	Y1998	F1999	D2001	D2002	S2002	G2003	V2004	D2005	K2006	V2007	G2008	T2010	E2011	D2012	D2013	G2014	E2021	N2022	G2023	E2024	N2025	Q2026	I2027	N2031	T2032	E2033	D2034	G2035	F2036	K2037			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41523	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 ($e^-/\text{\AA}^2$)	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	2.188	Depositor
Minimum map value	-0.441	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.504	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 [i](#)

5.1 Standard geometry [i](#)

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	0.16	0/19378	0.33	0/26233

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1037	ASP	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	19006	0	18363	296	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19007	0	18363	296	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.

The worst 5 of 296 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:1574:ASN:HD22	1:A:1686:SER:HB2	1.40	0.86
1:A:1035:ILE:HG23	1:A:1039:VAL:HG12	1.67	0.76
1:A:1172:MET:HE2	1:A:1191:PRO:HB2	1.68	0.74
1:A:2034:ASP:O	1:A:2037:LYS:NZ	2.21	0.73
1:A:968:LEU:HB3	1:A:985:MET:HG3	1.71	0.72

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	2361/2397 (98%)	2240 (95%)	118 (5%)	3 (0%)	48 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1036	ILE
1	A	1269	PHE
1	A	1069	VAL

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	2134/2163 (99%)	2087 (98%)	47 (2%)	45 63

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1093	LEU
1	A	1648	TYR
1	A	1111	LEU
1	A	1305	THR
1	A	1759	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1380	ASN
1	A	1472	ASN
1	A	2261	ASN
1	A	1413	ASN
1	A	1574	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

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

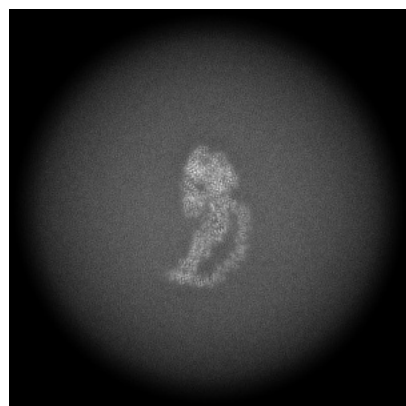
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18373. These allow visual inspection of the internal detail of the map and identification of artifacts.

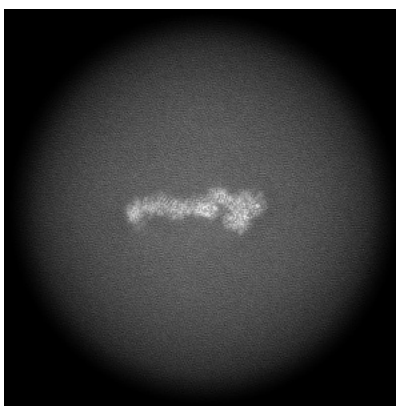
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

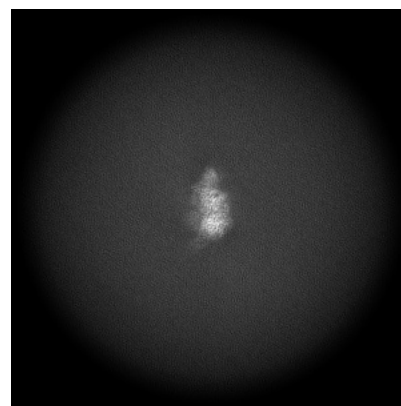
6.1.1 Primary map



X

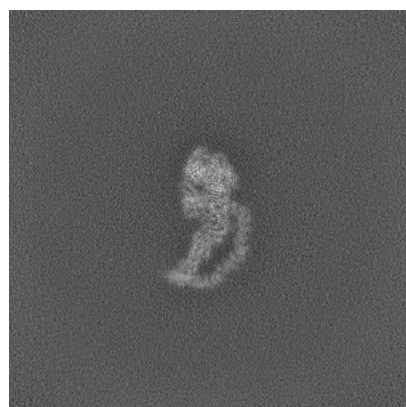


Y

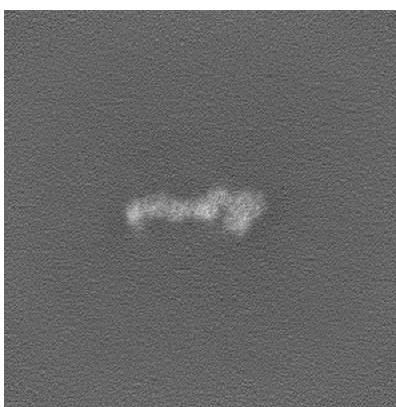


Z

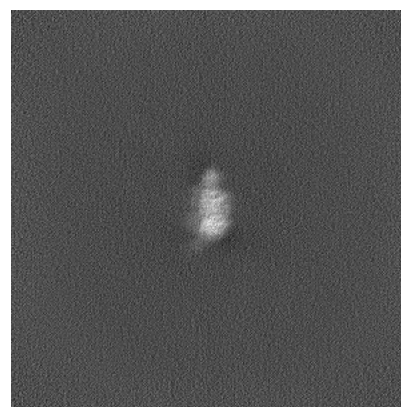
6.1.2 Raw map



X



Y

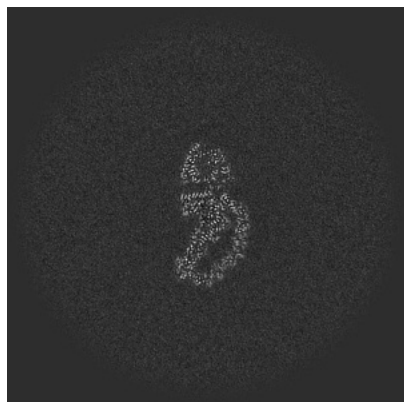


Z

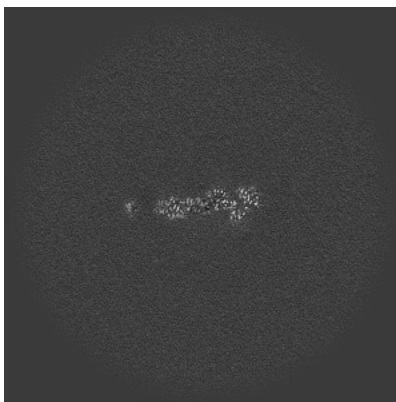
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

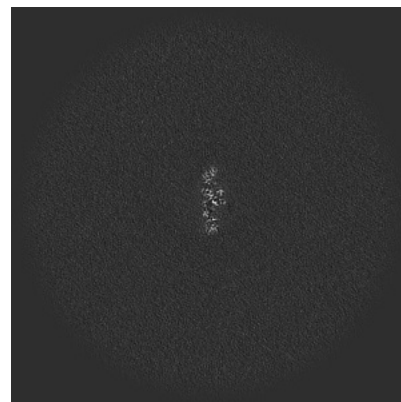
6.2.1 Primary map



X Index: 250

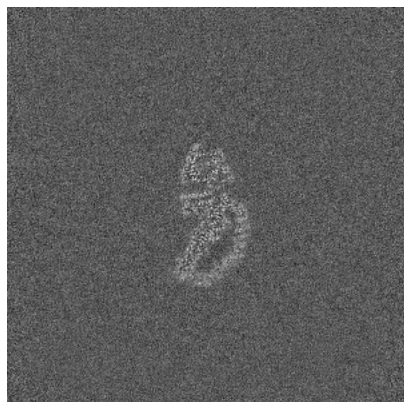


Y Index: 250

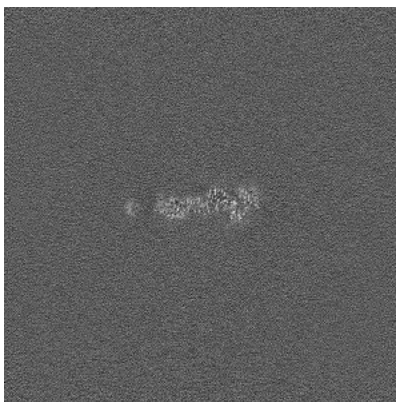


Z Index: 250

6.2.2 Raw map



X Index: 250



Y Index: 250

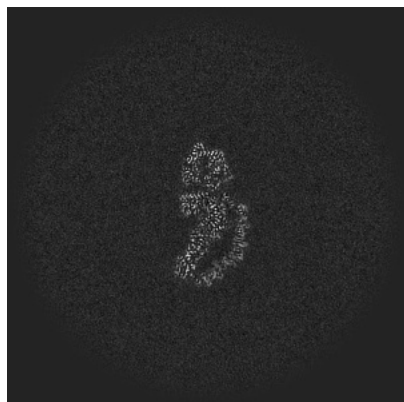


Z Index: 250

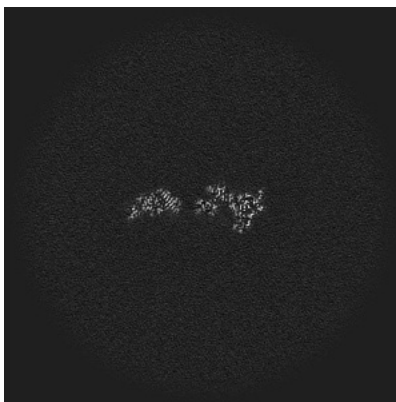
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

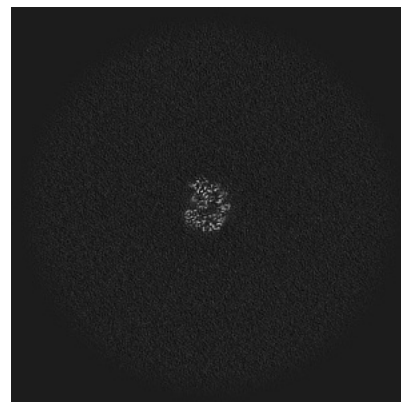
6.3.1 Primary map



X Index: 252

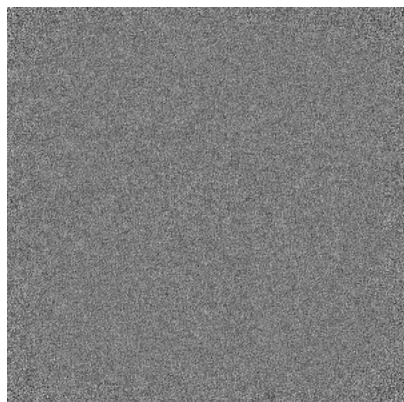


Y Index: 232

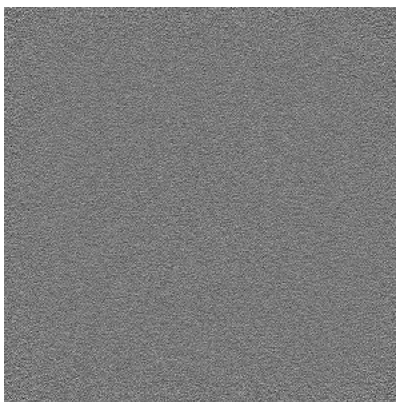


Z Index: 294

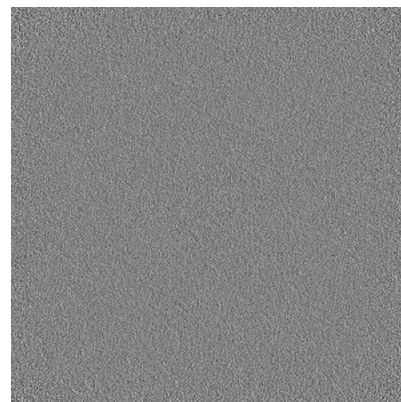
6.3.2 Raw map



X Index: 0



Y Index: 0

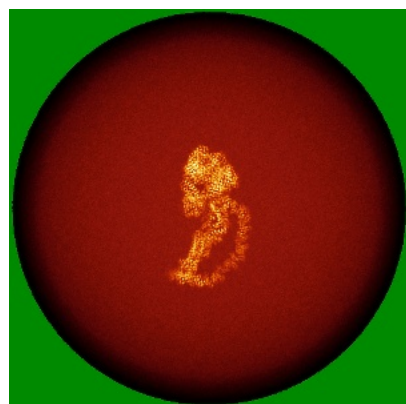


Z Index: 0

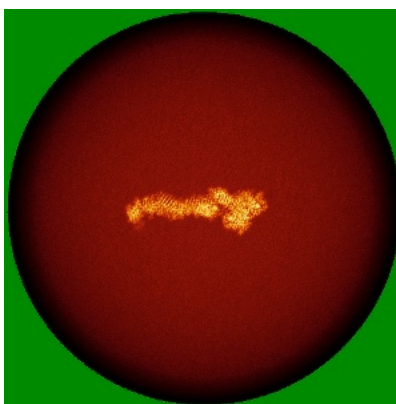
The images above show the largest variance slices of the map in three orthogonal directions.

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

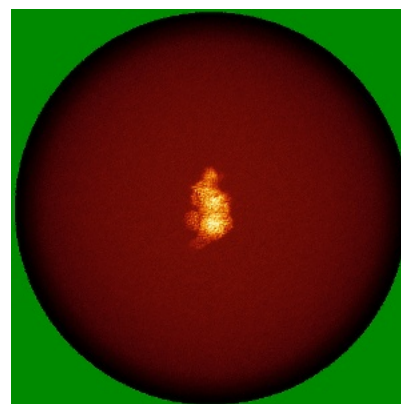
6.4.1 Primary map



X

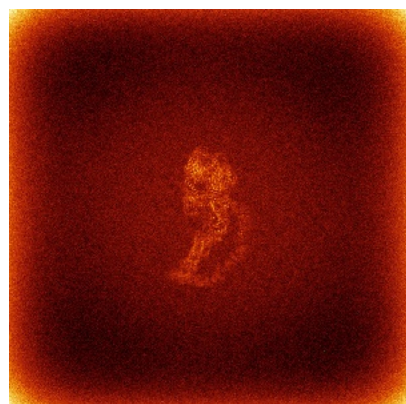


Y

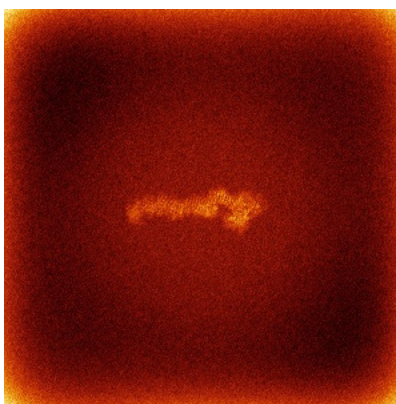


Z

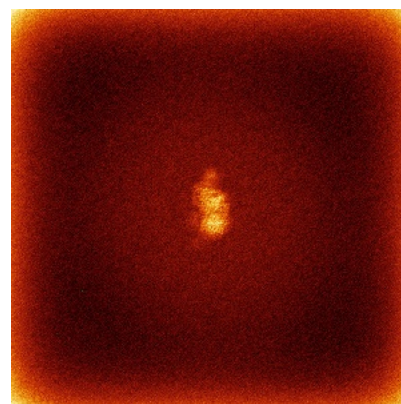
6.4.2 Raw map



X



Y

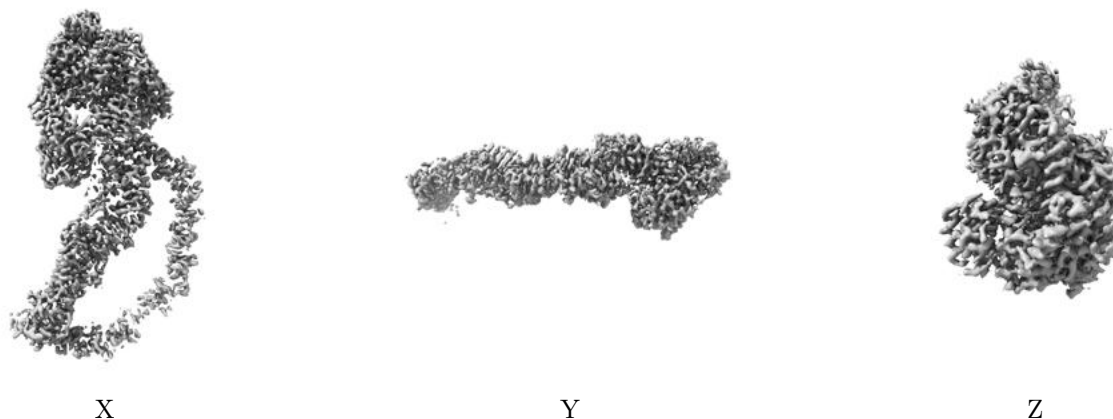


Z

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.

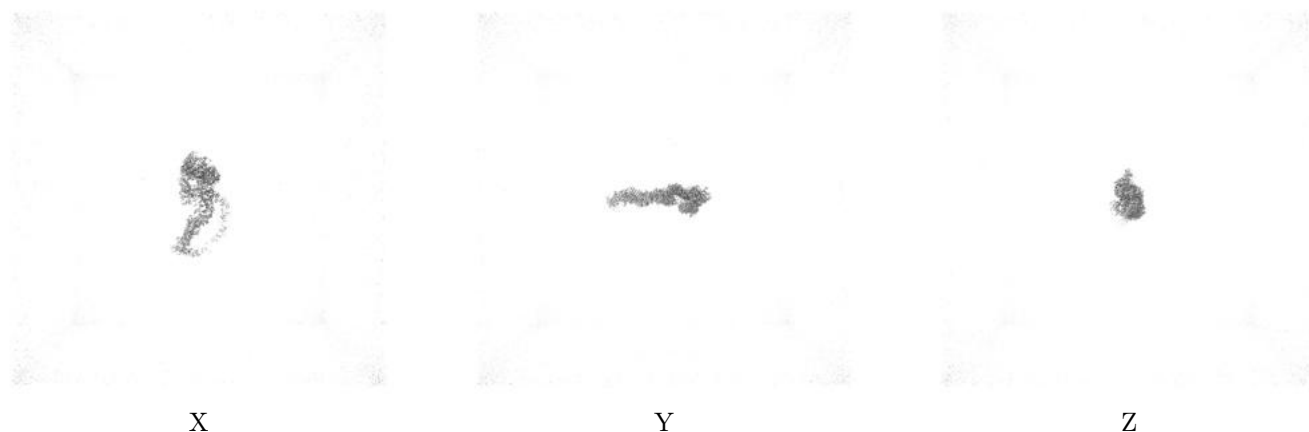
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.504. 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



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.

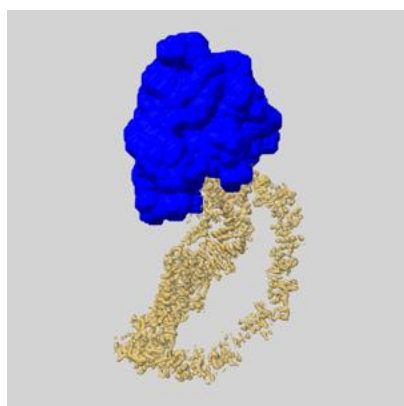
6.6 Mask visualisation [i](#)

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

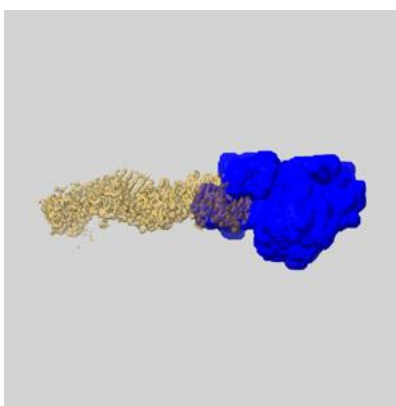
A mask typically either:

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

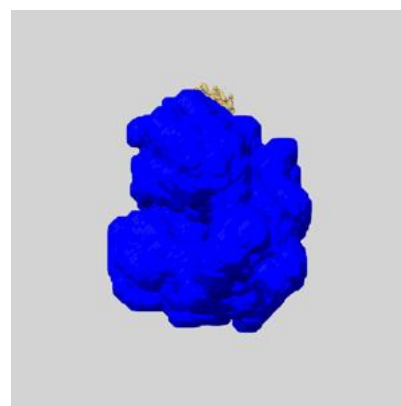
6.6.1 emd_18373_msk_1.map [i](#)



X

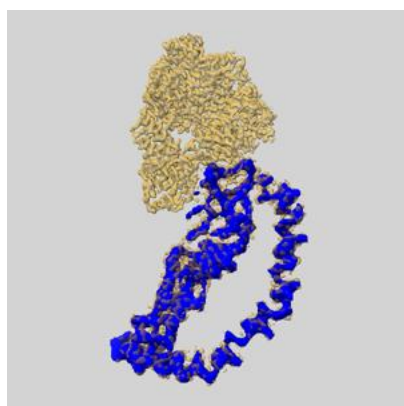


Y

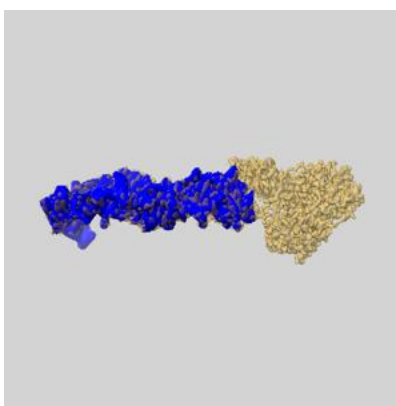


Z

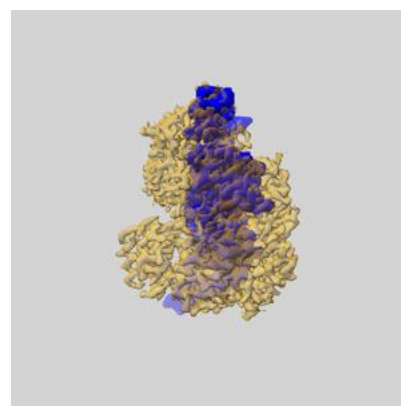
6.6.2 emd_18373_msk_2.map [i](#)



X



Y

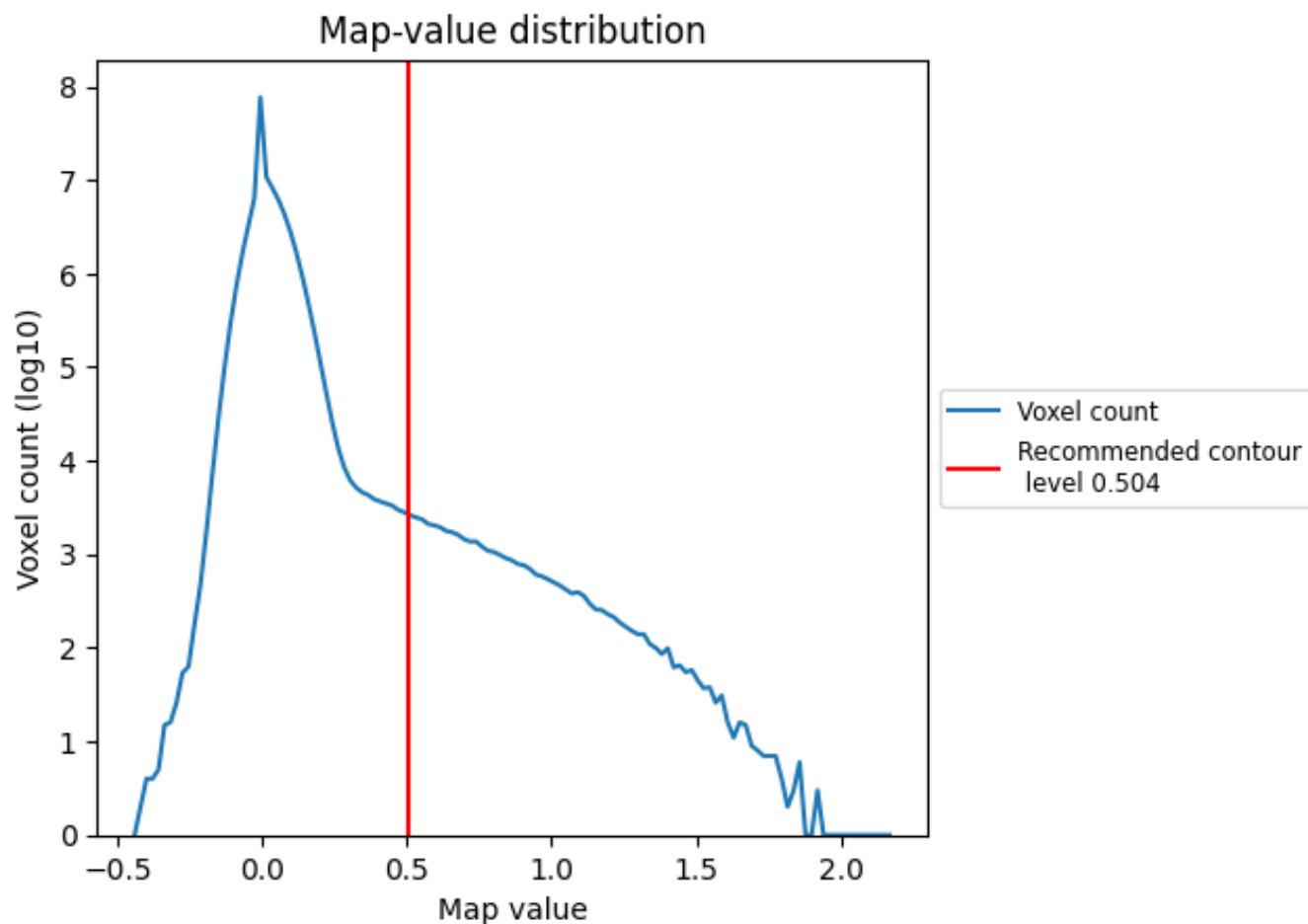


Z

7 Map analysis [i](#)

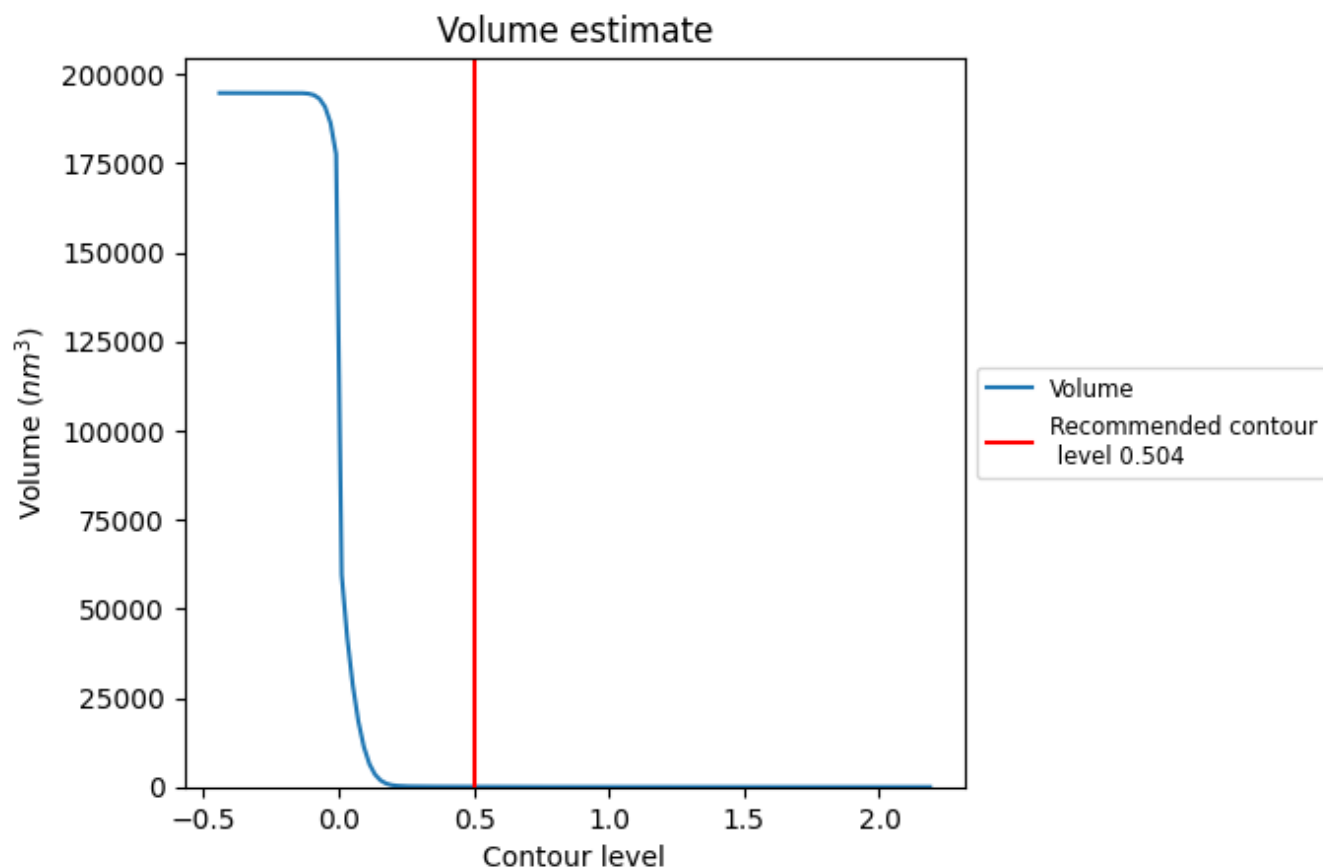
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

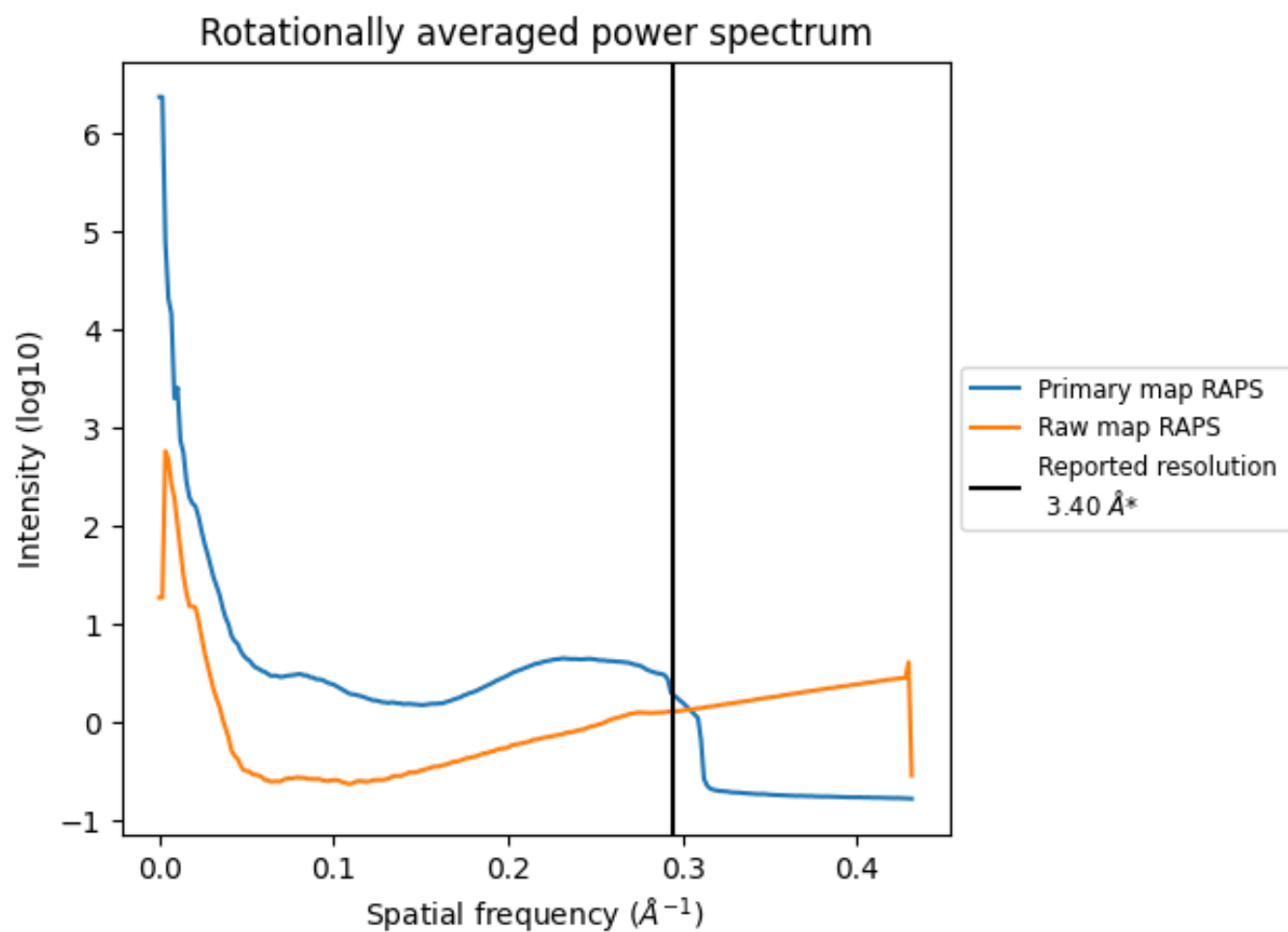
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 61 nm^3 ; this corresponds to an approximate mass of 55 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 ⓘ

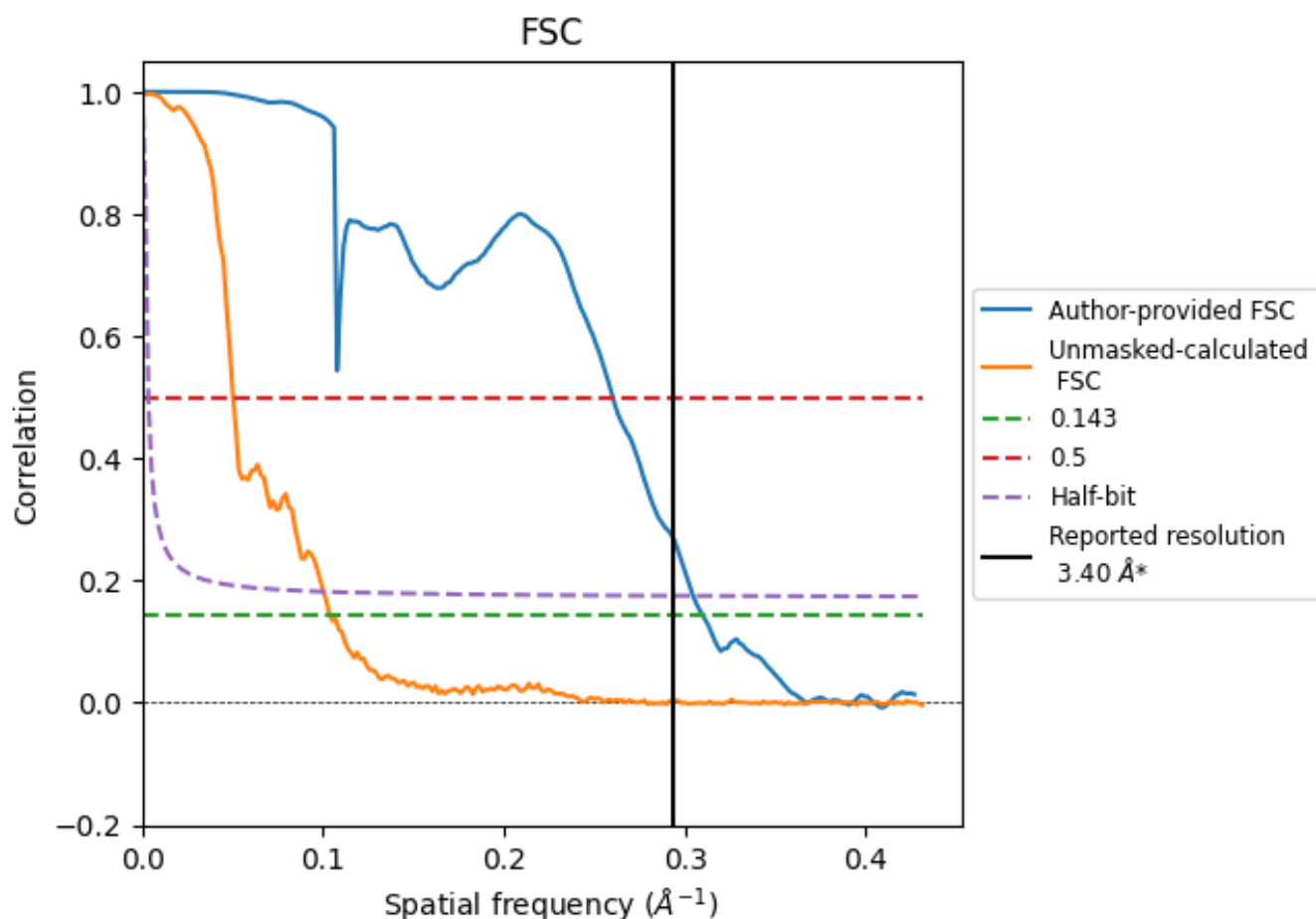


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

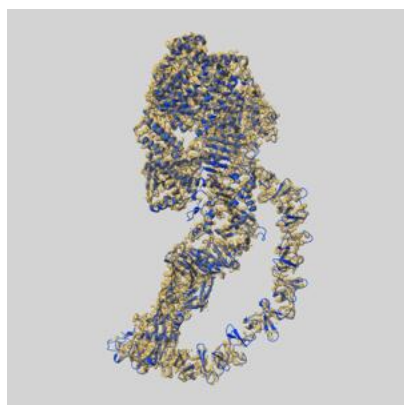
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.23	3.84	3.28
Unmasked-calculated*	9.62	19.88	9.98

*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 9.62 differs from the reported value 3.4 by more than 10 %

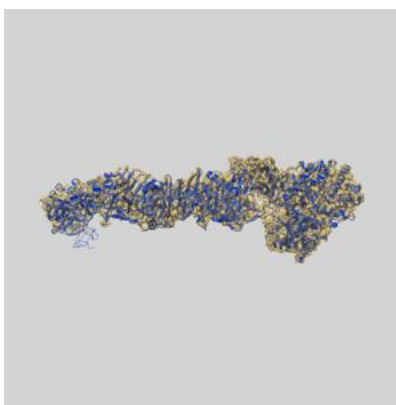
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18373 and PDB model 8QEN. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

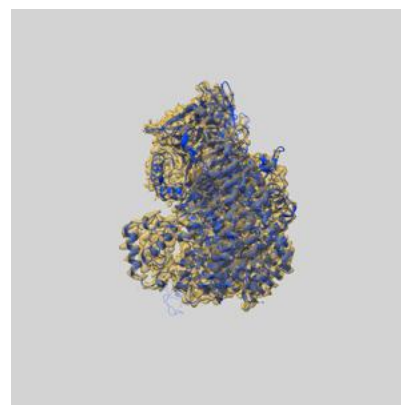
9.1 Map-model overlay [i](#)



X



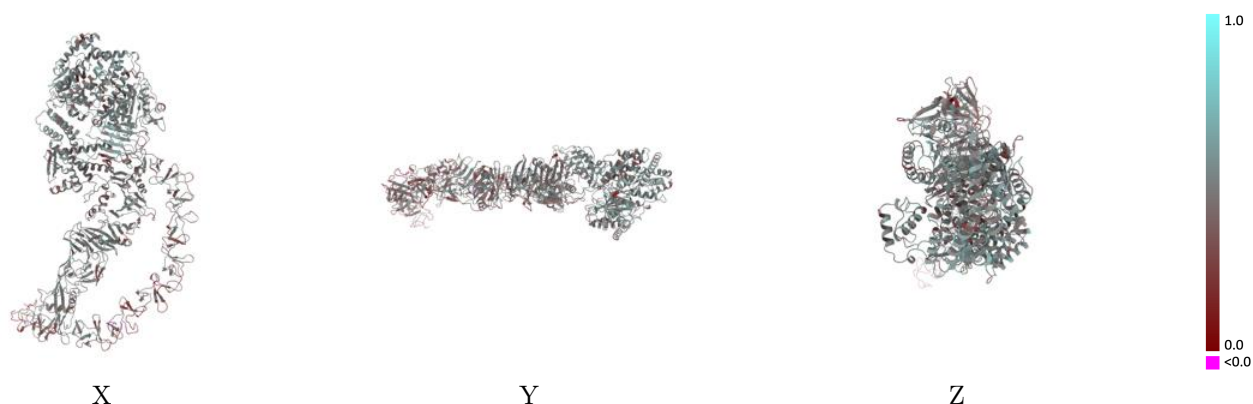
Y



Z

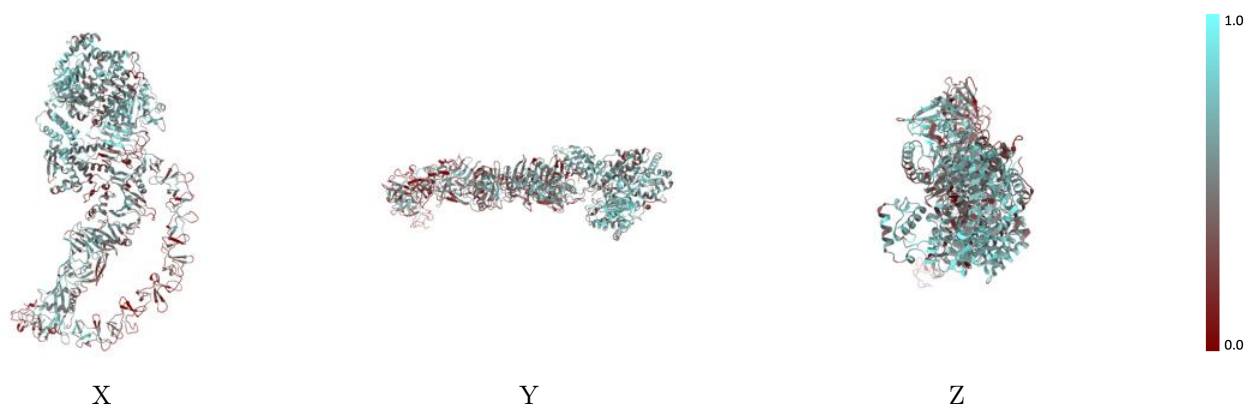
The images above show the 3D surface view of the map at the recommended contour level 0.504 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



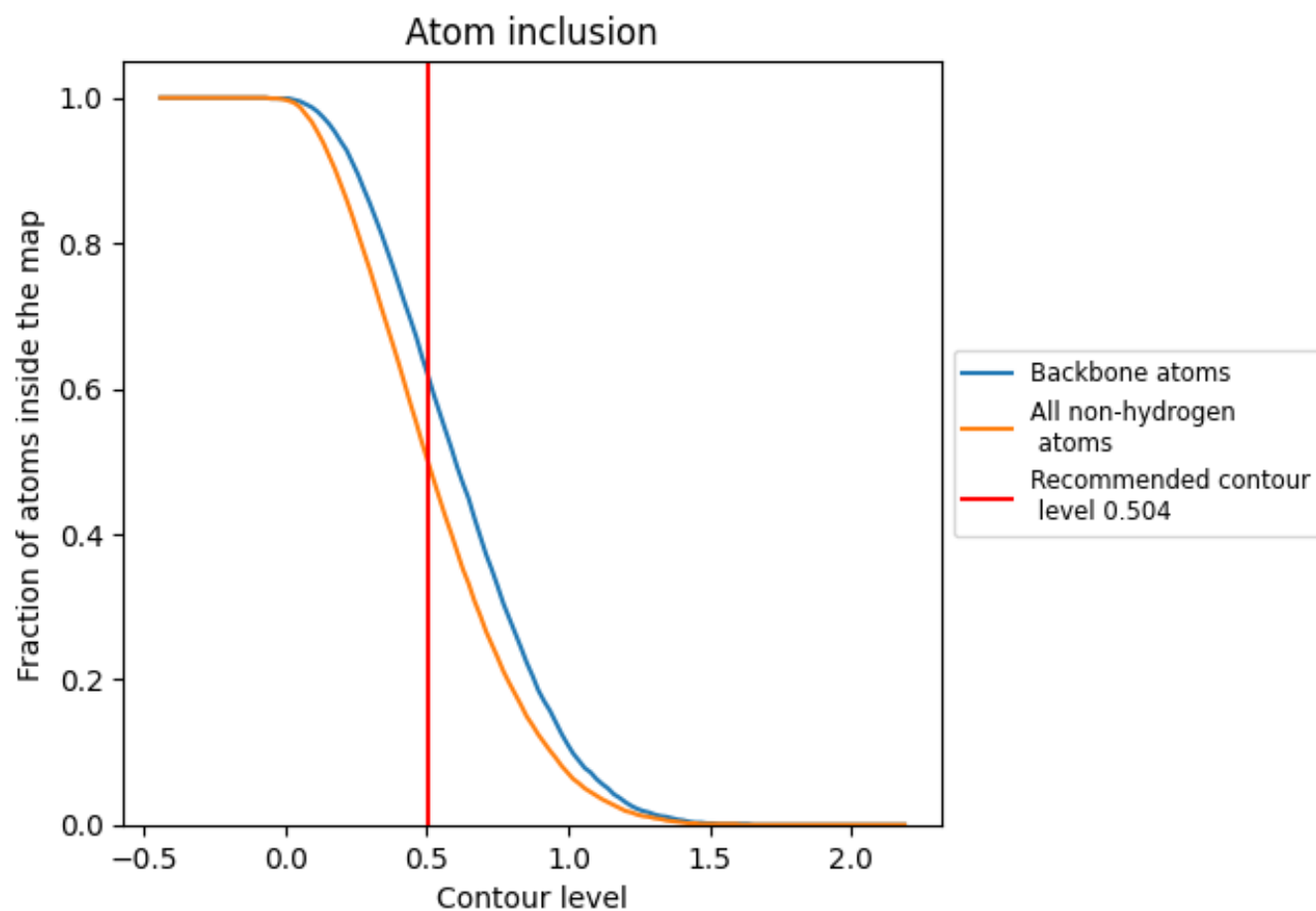
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.504).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 50% 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 (0.504) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4990	0.4520
A	0.4990	0.4520

