



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2024 – 01:56 PM EDT

PDB ID : 8EZ9
EMDB ID : EMD-28731
Title : Dimeric complex of DNA-PKcs
Authors : Chen, S.; He, Y.
Deposited on : 2022-10-31
Resolution : 5.67 Å(reported)

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.dev92
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) : 2.36.2

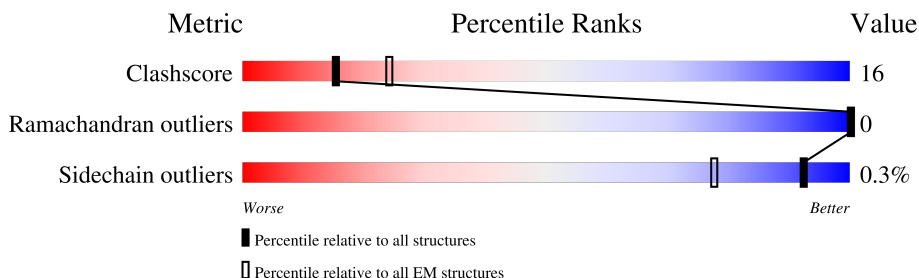
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.67 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 $\leq 5\%$. 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	Q	20	<div> <div>25%</div> <div>90%</div> <div>10%</div> </div>
1	R	20	<div> <div>25%</div> <div>90%</div> <div>10%</div> </div>
2	C	4128	<div> <div>30%</div> <div>58%</div> <div>30%</div> <div>11%</div> </div>
2	L	4128	<div> <div>31%</div> <div>59%</div> <div>30%</div> <div>11%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 58770 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 unknown region of DNA-PKcs.

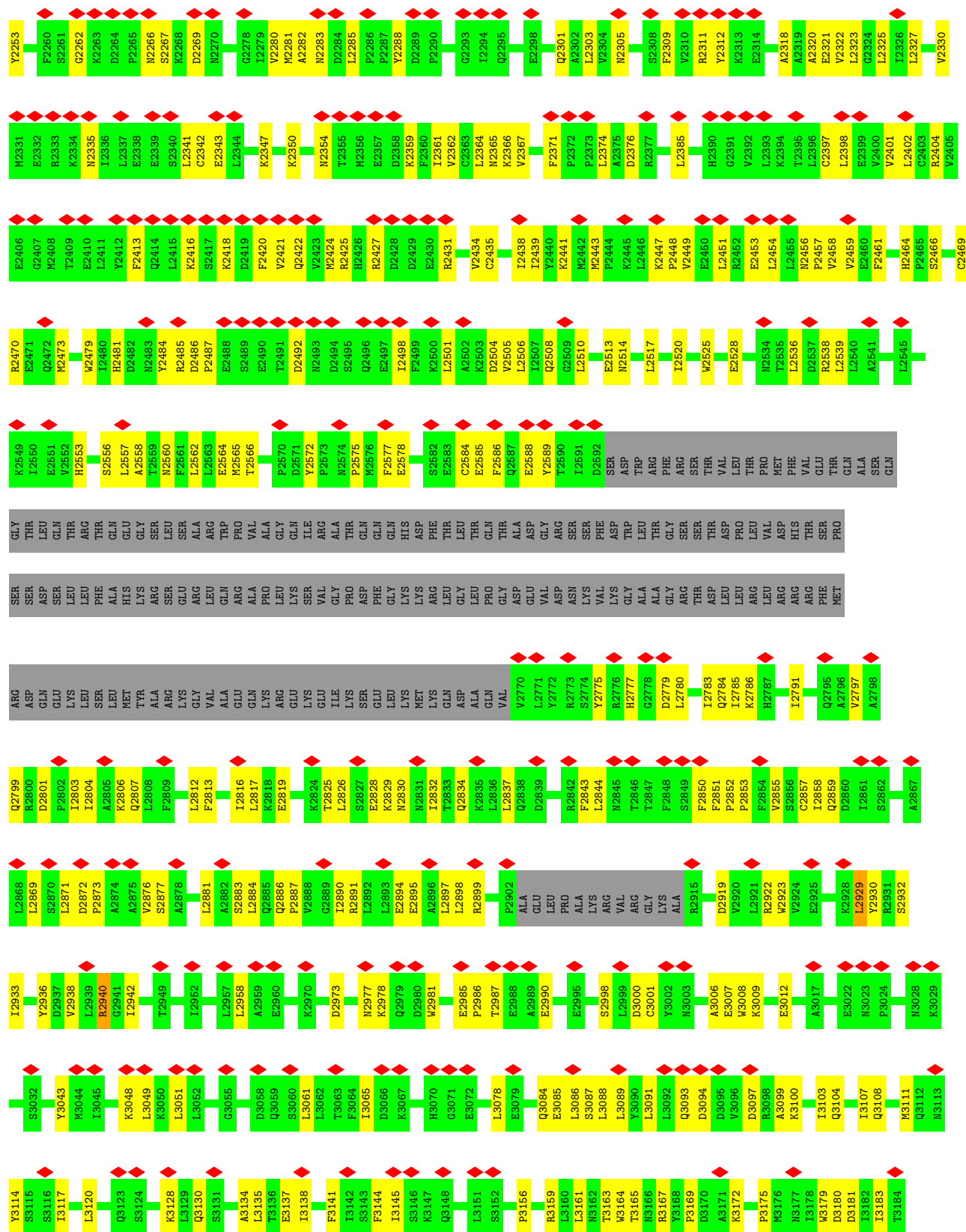
Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	20	Total	C	N	O	0	0
			101	60	20	21		
1	Q	20	Total	C	N	O	0	0
			101	60	20	21		

- Molecule 2 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	3662	Total	C	N	O	S	0	0
			29284	18776	4946	5370	192		
2	C	3662	Total	C	N	O	S	0	0
			29284	18776	4946	5370	192		

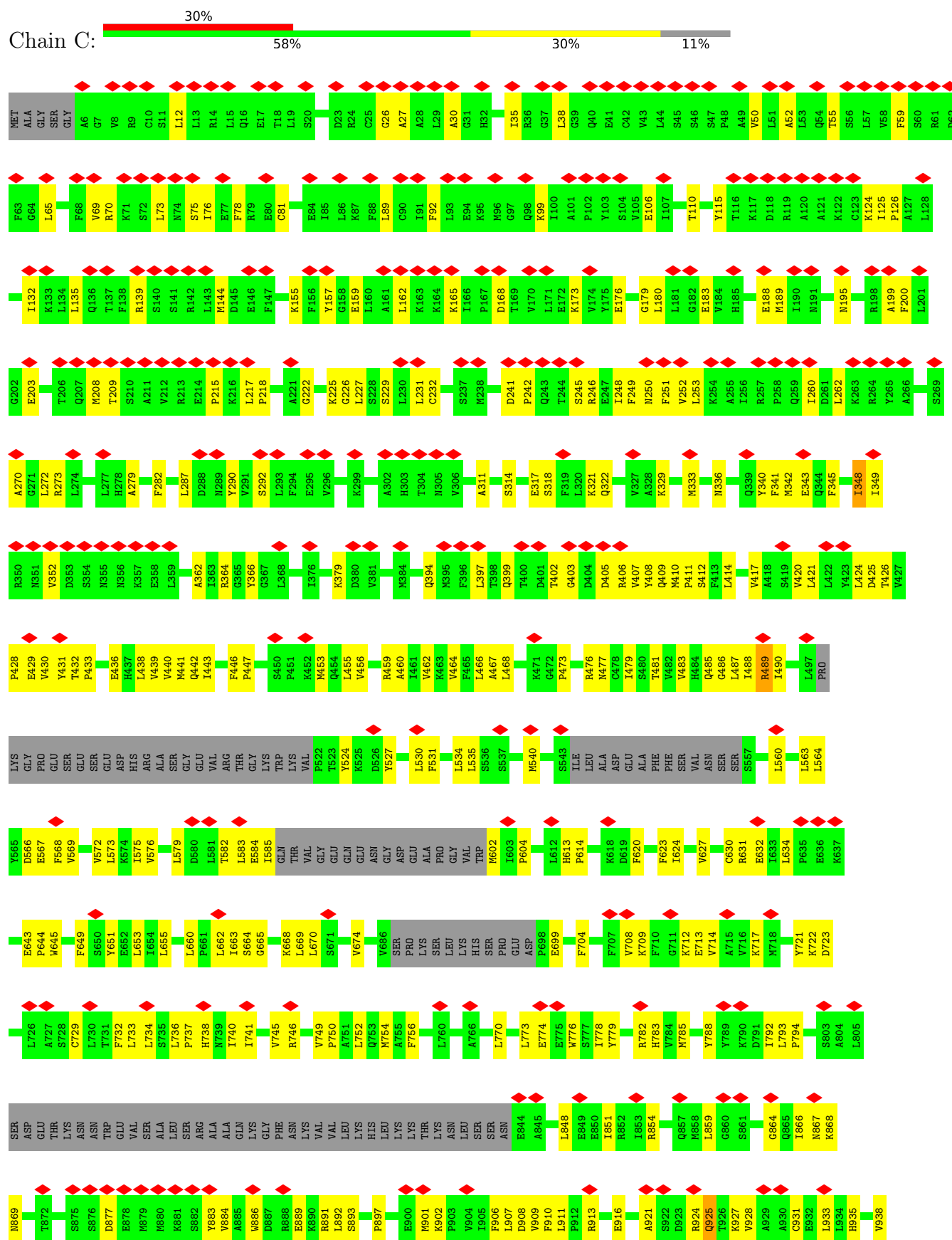


N2177	G2178	G2179	G2180	G2181	T2182	H2183	Y2184	N2185	V2190	L2193	T2197	G2198	L2199	A2200	T2201	P2202	T2203	G2204	V2205	P2206	K2207	D2208	E2209	L2210	N2141	T2142	A2212	N2213	L2216	N2217	F2218	L2219	N2220	V2223	F2224	H2225	R2228	A2229	V2230	E2236	L2237	T2240	L2241	N2242	E2243	C2244	V2245	K2246	D2247	C2248	L2249					
L2108	GLY	PRO	PRO	GLN	GLY	GLU	GLU	ASP	SER	VAL	P2119	R2120	D2121	L2122	P2123	S2124	W2125	K2132	L2133	G2134	N2135	P2136	L2137	V2138	P2139	L2140	N2141	E2142	L2143	L2144	F2145	L2146	A2147	K2148	L2149	V2150	L2151	N2152	T2153	E2154	E2155	V2156	F2157	R2158	P2159	W2164	L2165	L2168	L2169	Q2170	L2171	A2172	A2173	S2174	E2175	N2176
SER	THR	GLY	ASN	PHE	PRO	VAL	VAL	SER	THR	GLU	VAL	GLU	VAL	GLU	VAL	GLN	ASP	PRO	ARG	ALA	LYS	THR	GLY	ARG	PHE	ARG	ARG	GLU	GLN	ARG	ASP	THR	GLU	LEU	SER	LEU	SER	THR	VAL	GLU	SER	GLN	PHE	ASP	PHE	H2105	R2106	S2107								
M2085	D2086	E2087	R2090	H2091	E2092	M2094	A2095	P2096	L2097	T2098	A2099	L2100	V2101	K2102	H2105	R2106	S2107																																							
L2151	N2152	T2153	E2154	E2155	V2156	F2157	R2158	P2159	W2164	L2165	L2168	L2169	Q2170	L2171	A2172	A2173	S2174	E2175	N2176																																					
K1422	I1423	T1424	A1425	Q1426	S1427	I1428	E1429	E1430	K1431	C1432	A1433	V1434	N1435	L1436	Y1437	Q1438	P1439	D1440	A1441	Q1442	D1443	R1444	R1445	L1448	L1464	H1465	N1466	I1467	L1468	P1469	S1470	Q1471	S1472	T1473	L1475	H1476	L1477	F1478	S1479	K1489	G1490	I1491	A1492	P1493	G1494	D1495	E1496	R1497	Q1498							





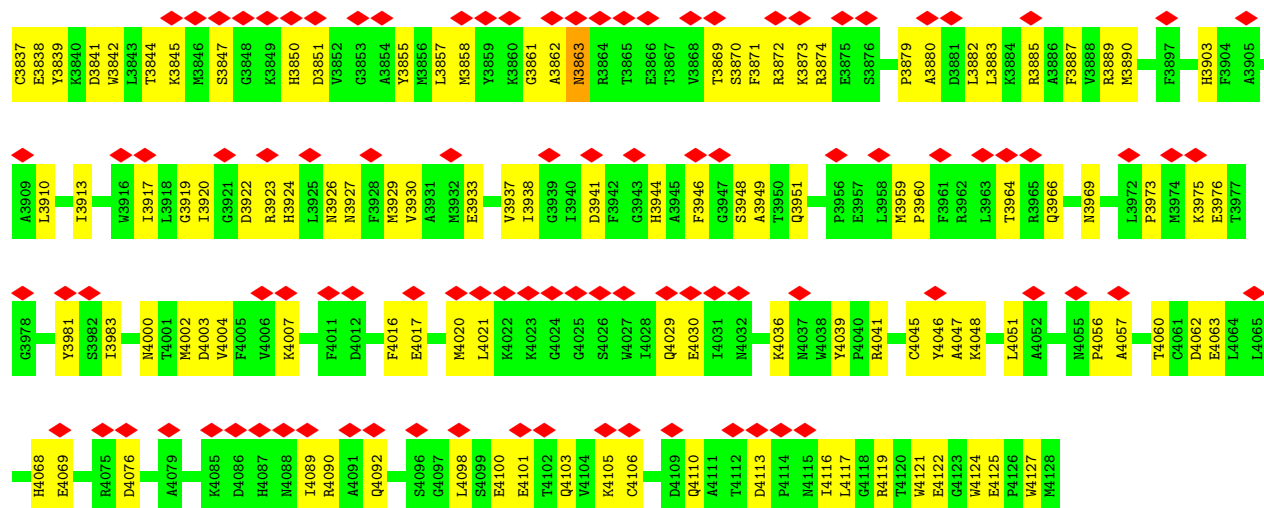
• Molecule 2: DNA-dependent protein kinase catalytic subunit



L1858	L1859	E1860	S1861	T1862	F1863	D1864	T1865	Q1866	T1867	K1868	D1806	K1807	D1808	D1809	P1810	R1811	L1812	L1813	K1814	T1815	R1816	Q1817	S1818	F1819	D1820	D1821	R1822	S1823	L1824	L1825	L1828	W1829	H1830	C1831	S1832	L1833	D1834	A1835	L1836	R1837	E1838	F1839	F1840	S1841	T1842	T1843	V1844	V1845	D1846	A1847	L1848	D1849	V1850	L1851	K1852	S1853	R1854	F1855	T1856	K1857
L1793	Q1794	V1795	G1796	L1797	L1798	M1804	F1805	R1806	K1807	D1808	D1809	P1810	R1811	L1812	L1813	F1814	T1815	R1816	Q1817	S1818	F1819	D1820	D1821	R1822	S1823	L1824	L1825	L1828	W1829	H1830	C1831	S1832	L1833	D1834	A1835	L1836	R1837	E1838	F1839	F1840	S1841	T1842	T1843	V1844	V1845	D1846	A1847	L1848	D1849	V1850	L1851	K1852	S1853	R1854	F1855	T1856	K1857			
S1726	R1727	E1728	F1729	P1730	P1731	G1732	T1733	F1736	N1737	V1740	D1741	C1742	M1743	K1744	K1745	F1746	L1747	D1748	A1749	L1750	S1755	F1756	M1757	L1758	L1759	E1760	L1761	M1762	T1763	E1764	V1765	L1766	C1767	R1768	E1769	Q1770	Q1771	E1775	E1776	L1777	F1778	Q1779	S1780	S1781	F1782	R1783	R1784	L1785	A1786	R1787	R1788	G1789	S1790	C1791	V1792					
L1649	A1650	K1651	L1652	L1653	Q1654	T1655	D1656	S1657	S1658	V1659	M1662	T1663	S1664	H1665	L1666	S1667	E1670	T1673	V1674	F1675	L1676	F1677	I1678	L1679	A1680	D1681	T1682	D1685	L1688	K1689	L1690	V1693	T1703	S1706	L1707	E1708	L1709	L1710	R1711	R1712	V1713	L1714	E1715	Q1716	L1717	L1718	V1719	F1722	P1723	M1724	Q1725									
L1572	L1575	V1579	L1580	Q1584	S1585	D1588	M1592	V1593	V1596	L1597	M1598	L1601	D1602	Q1603	F1604	F1605	R1606	R1608	A1609	A1610	A1611	Q1614	K1617	L1618	A1619	L1623	Q1624	K1628	C1629	D1630	S1631	V1632	V1633	A1634	K1635	D1636	S1637	P1638	L1639	K1642	M1643	L1646	A1647	L1648																
E1496	R1497	Q1498	C1499	L1500	P1501	S1502	D1504	L1505	L1515	F1519	G1522	G1523	L1524	R1527	L1528	L1531	L1532	L1533	M1534	P1535	A1536	V1537	L1538	S1539	T1540	ALA	SER	LEU	GLY	SER	GLN	GLY	S1549	V1550	I1551	H1552	F1553	S1554	G1555	G1556	E1557	V1558	F1559	Y1560	S1561	L1562	F1563	S1564	I1567	M1568	T1569									
E1416	T1417	H1418	K1422	L1423	T1424	A1425	Q1426	S1427	L1428	E1429	E1430	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	G1438	D1440	A1441	Q1442	V1443	D1444	R1445	L1448	V1452	K1456	H1459	L1464	H1465	N1466	L1467	L1468	P1469	S1470	Q1471	S1472	L1475	H1476	H1477	S1478	K1489	G1490	L1491	A1492	L1493	G1494	D1495											
ALA	GLY	ASN	ARG	THR	S1323	P1324	Q1325	F1326	G1327	E1328	R1329	V1330	M1331	L1332	S1333	K1334	C1335	T1336	L1337	V1338	V1339	R1340	T1341	M1342	E1343	T1346	L1347	L1348	L1349	M1350	L1359	M1365	T1366	H1367	L1368	M1369	R1370	V1371	L1372	L1376	C1377	E1378	P1379	A1380	S1381	F1384	N1385	I1386	G1387	D1388	V1389	Q1390	L1391	M1392						
PRO	PHE	S1249	L1250	Q1251	A1252	L1260	L1261	A1262	E1265	C1266	Y1267	N1268	F1269	F1270	L1271	G1272	E1273	R1274	T1275	V1276	G1277	A1278	V1281	L1282	G1283	T1284	E1285	A1286	Q1287	S1288	S1289	L1290	L1291	K1292	A1293	V1294	L1298	E1299	A1302	M1303	H1304	I1306	I1307	A1308	A1309	E1310	K1311	CYS	PHE	GLY	THR	GLY	ALA							
H1175	C1176	G1177	R1178	P1179	Q1180	T1181	E1182	L1183	R1184	H1185	T1188	F1191	F1194	V1195	L1196	L1197	L1198	P1199	G1200	S1203	P1204	N1205	L1206	W1207	L1208	L1209	D1210	V1211	L1212	K1213	E1214	E1215	F1219	N1222	T1223	F1224	E1225	G1226	C1229	S1233	A1237	Q1238	P1239	T1240	L1241	L1242	Y1243	ARG	GLY											
F1101	E1102	A1103	L1104	V1105	T1106	M1107	L1108	L1111	A1112	L1113	A1116	D1117	E1118	K1119	S1120	T1124	Q1125	T1131	H1132	L1133	C1135	R1136	T1137	T1138	H1142	L1145	M1146	K1147	A1148	K1149	K1150	R1151	R1155	G1156	F1157	P1158	P1159	S1160	A1161	S1162	G1164	L1165	L1166	D1167	V1168	V1169	K1170	L1173	A1174											
V1021	D1022	S1023	T1024	L1025	R1026	F1036	L1037	K1041	Q1043	T1044	A1045	P1046	Q1047	Q1048	Q1049	Q1050	K1051	P1053	V1054	N1055	S1058	K1061	R1062	L1063	Y1064	S1065	L1066	A1067	L1068	H1069	A1072	R1075	L1076	G1077	A1078	A1081	N1084	I1085	Y1086	L1010	E1011	A1012	E1013	L1014	T1017	V1018	D1019	F1099	V1100											
H939	F940	H941	Q947	M948	P949	E950	G951	Q952	Q953	G954	A955	P956	P957	H958	Q960	Y962	K963	R964	T965	D975	V976	V979	Q982	L983	Y984	E985	V988	L991	T992	H993	N997	E1002	S1003	Q1004	D1005	T1006	V1007	A1008	L1009	L1010	E1011	A1012	E1013	L1014	T1017	V1018	D1019	F1099	V1100											







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	356.6592, 356.6592, 356.6592	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8256, 0.8256, 0.8256	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	$\# Z > 5$
2	C	0.30	0/29884	0.61	9/40387 (0.0%)
2	L	0.30	0/29884	0.61	8/40387 (0.0%)
All	All	0.30	0/59768	0.61	17/80774 (0.0%)

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
2	C	0	3
2	L	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2929	LEU	CB-CG-CD2	-7.05	99.01	111.00
2	L	139	ARG	NE-CZ-NH2	7.04	123.82	120.30
2	L	2929	LEU	CB-CG-CD2	-7.04	99.03	111.00
2	C	139	ARG	NE-CZ-NH2	7.02	123.81	120.30
2	C	746	ARG	CA-CB-CG	5.94	126.47	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	364	ARG	Sidechain
2	C	366	TYR	Sidechain
2	C	489	ARG	Sidechain
2	L	364	ARG	Sidechain

Continued on next page...

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Mol	Chain	Res	Type	Group
2	L	489	ARG	Sidechain

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	Q	101	0	25	3	0
1	R	101	0	25	3	0
2	C	29284	0	29680	975	0
2	L	29284	0	29680	981	0
All	All	58770	0	59410	1928	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 16.

The worst 5 of 1928 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)
2:L:3606:ILE:O	2:L:3610:TYR:HB2	1.53	1.08
2:C:3606:ILE:O	2:C:3610:TYR:HB2	1.53	1.07
2:L:26:GLY:C	2:C:76:ILE:HD12	1.84	0.97
2:L:76:ILE:HD12	2:C:26:GLY:C	1.86	0.96
2:C:2890:ILE:HG12	2:C:2929:LEU:HD21	1.47	0.95

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	
2	C	3632/4128 (88%)	3344 (92%)	288 (8%)	0	100	100
2	L	3632/4128 (88%)	3343 (92%)	289 (8%)	0	100	100
All	All	7264/8256 (88%)	6687 (92%)	577 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
2	C	3266/3671 (89%)	3255 (100%)	11 (0%)	92	94
2	L	3266/3671 (89%)	3255 (100%)	11 (0%)	92	94
All	All	6532/7342 (89%)	6510 (100%)	22 (0%)	92	94

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1527	ARG
2	C	2485	ARG
2	C	2158	ARG
2	C	2940	ARG
2	L	2485	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	2301	GLN
2	C	3249	GLN
2	C	2305	ASN
2	C	3104	GLN
2	C	3634	GLN

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.

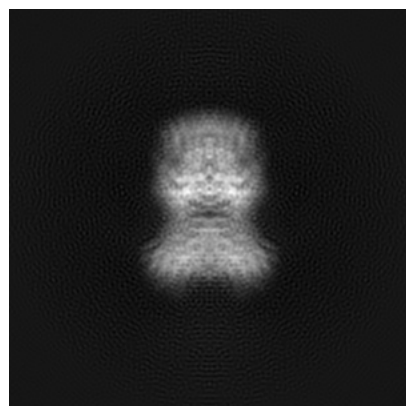
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28731. These allow visual inspection of the internal detail of the map and identification of artifacts.

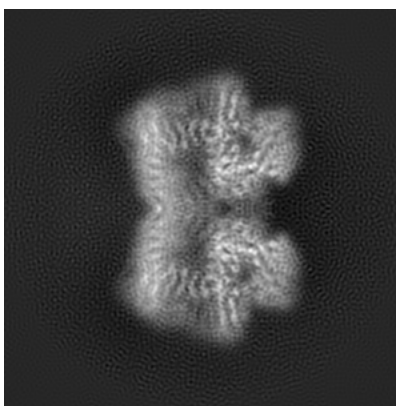
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

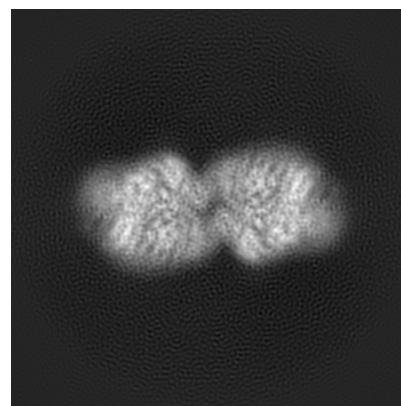
6.1.1 Primary map



X

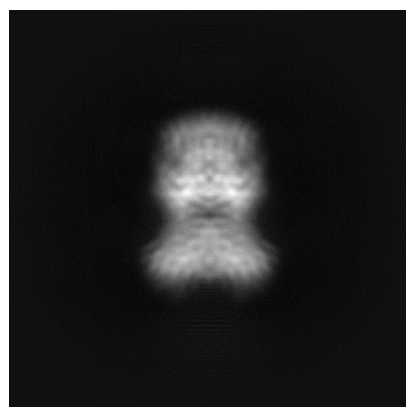


Y

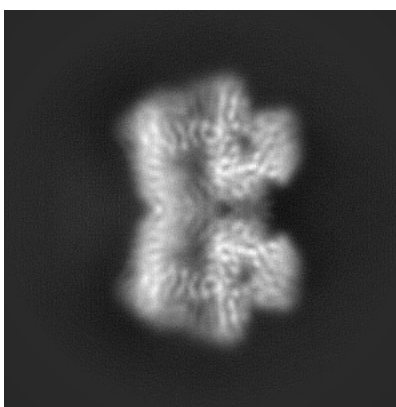


Z

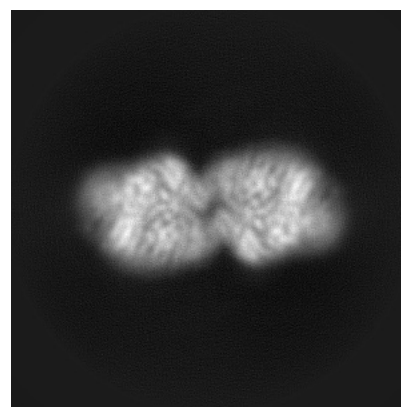
6.1.2 Raw map



X



Y

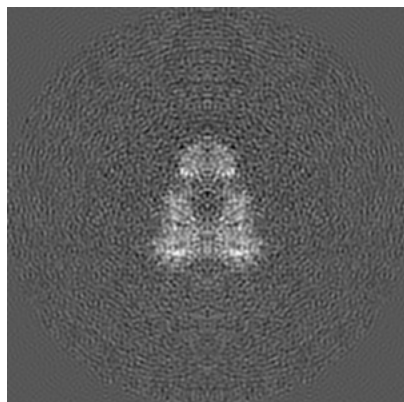


Z

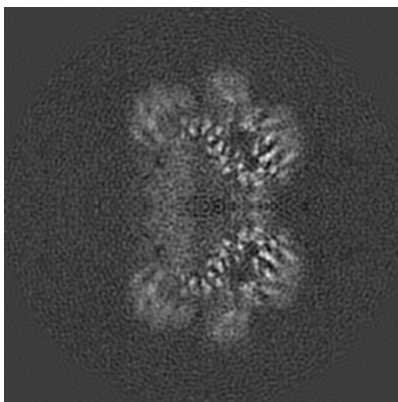
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

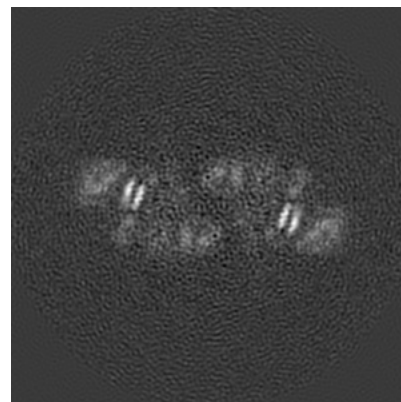
6.2.1 Primary map



X Index: 216

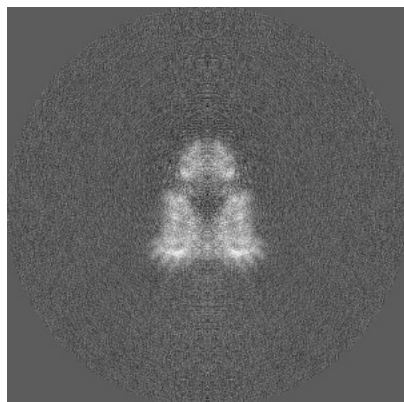


Y Index: 216

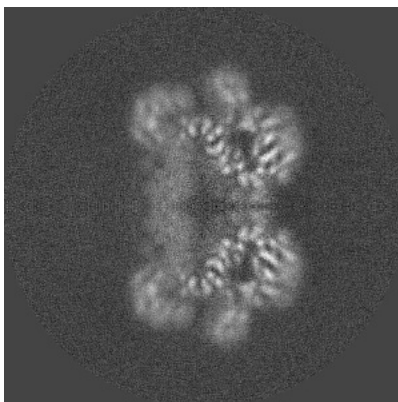


Z Index: 216

6.2.2 Raw map



X Index: 216



Y Index: 216

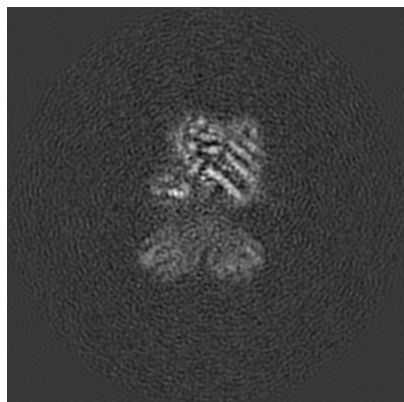


Z Index: 216

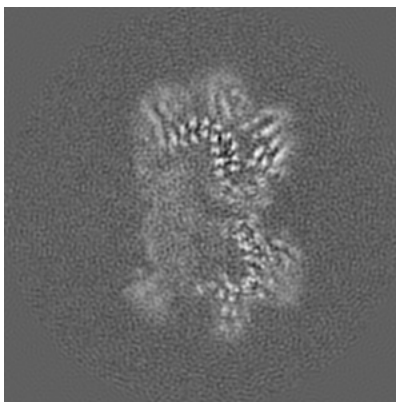
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

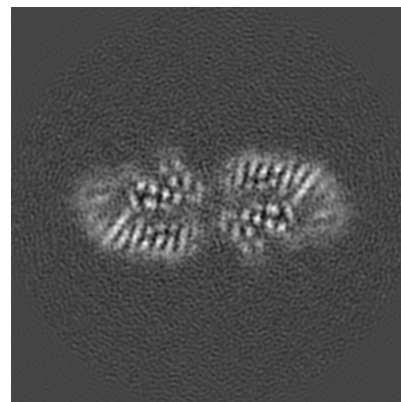
6.3.1 Primary map



X Index: 174

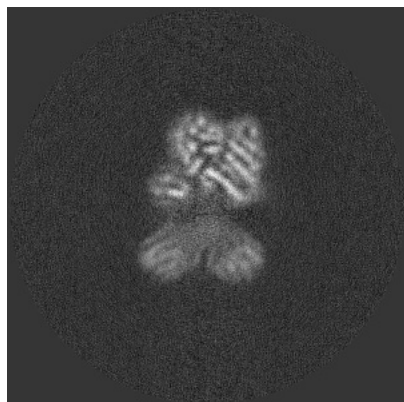


Y Index: 204

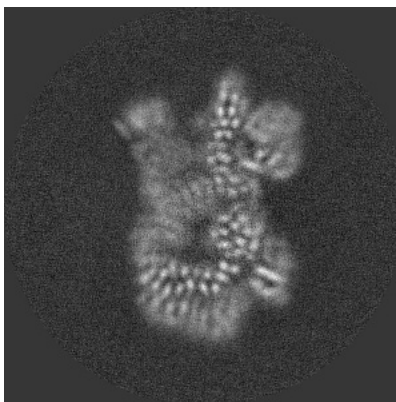


Z Index: 234

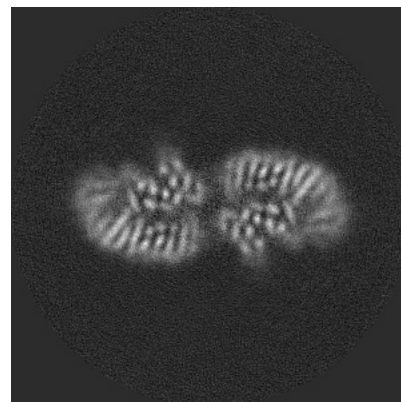
6.3.2 Raw map



X Index: 174



Y Index: 239

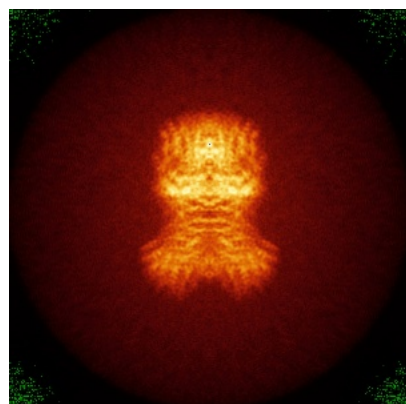


Z Index: 234

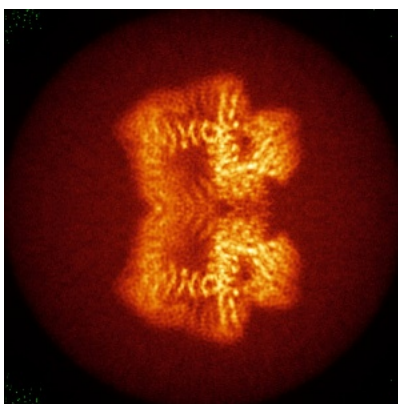
The images above show the largest variance slices of the map in three orthogonal directions.

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

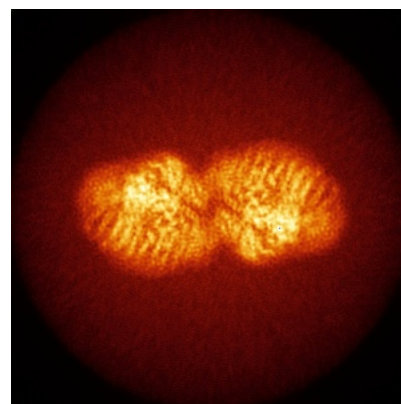
6.4.1 Primary map



X

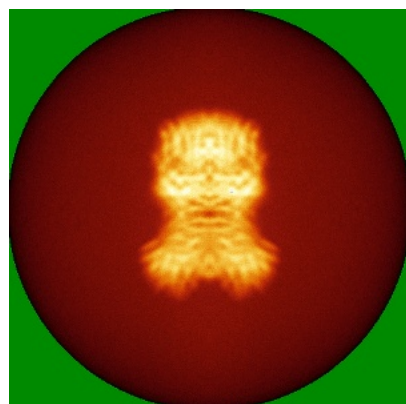


Y

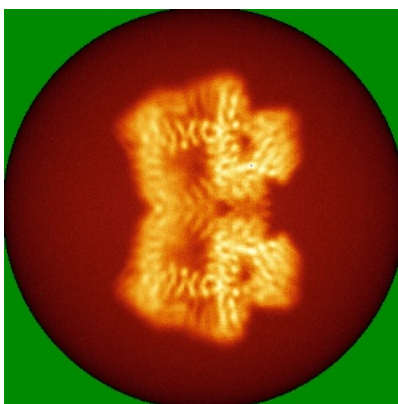


Z

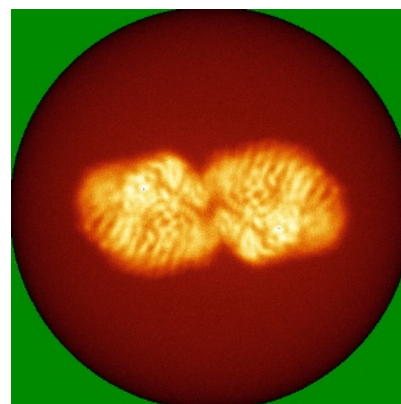
6.4.2 Raw map



X



Y

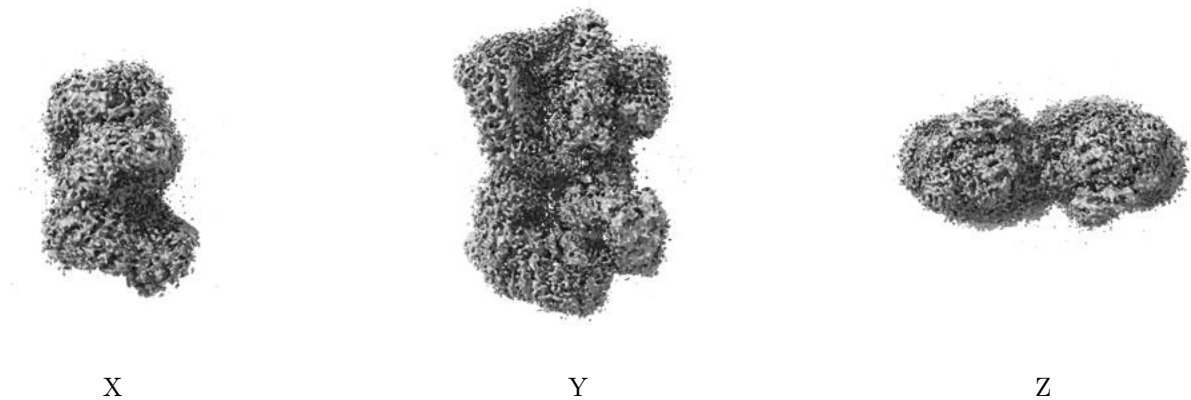


Z

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.

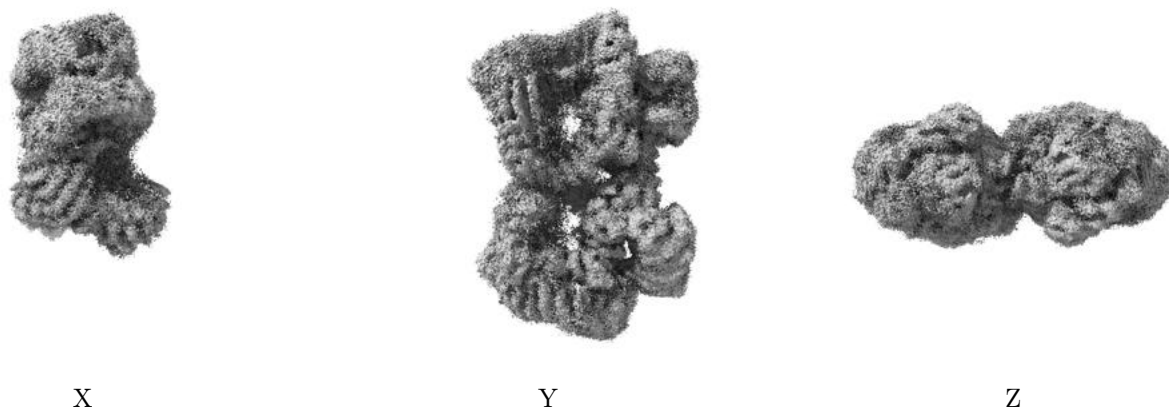
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

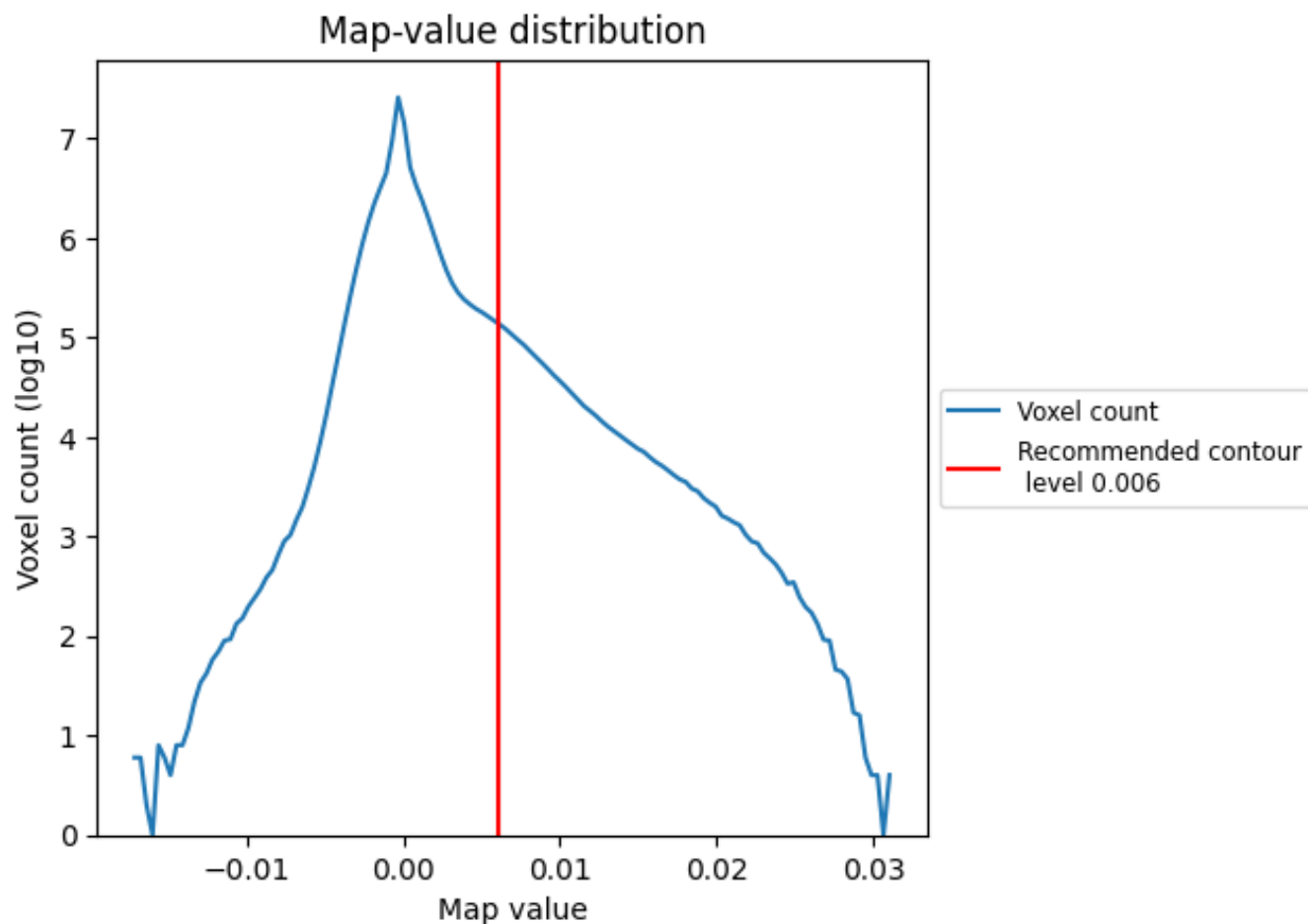
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

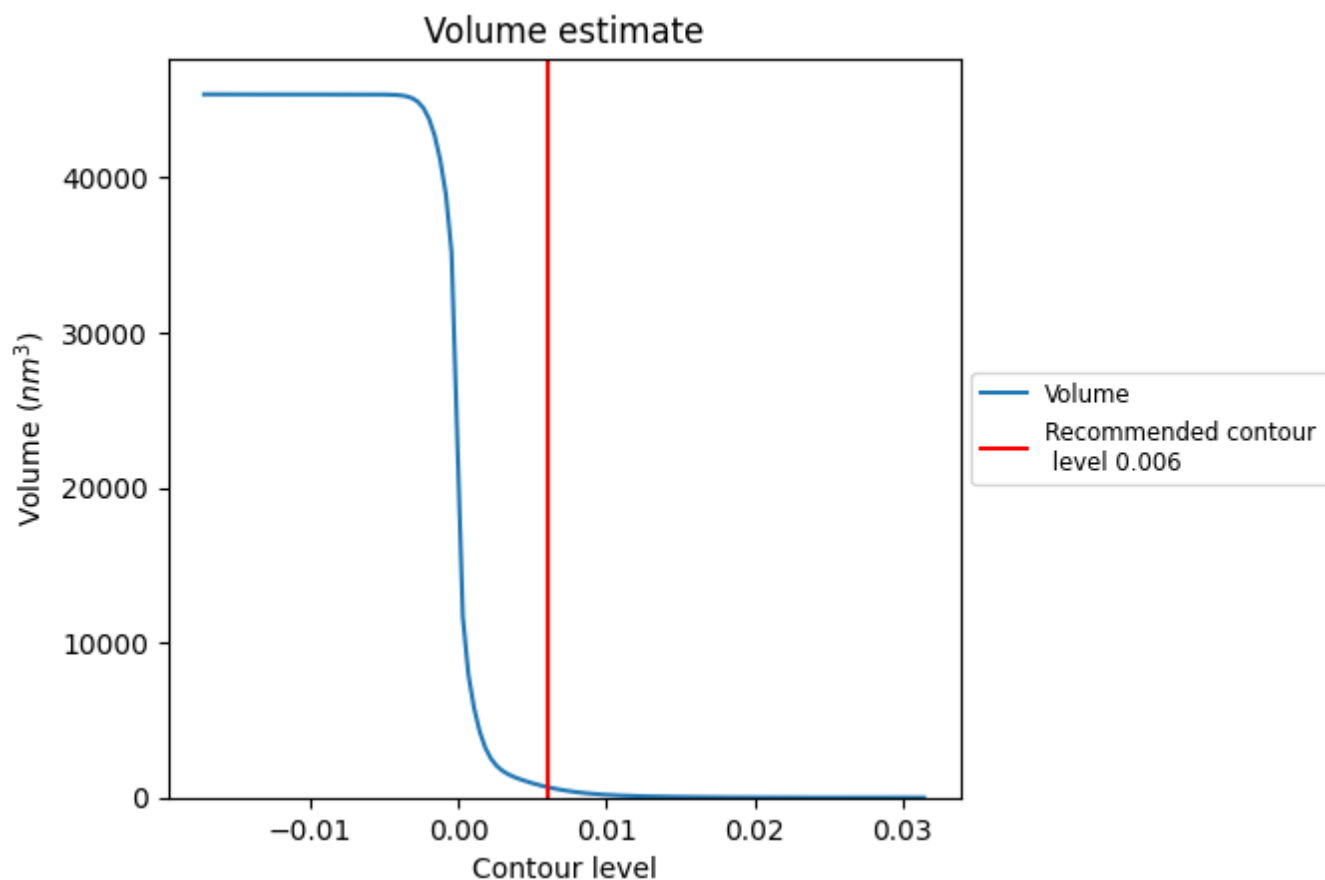
This section contains the results of statistical analysis of the map.

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.

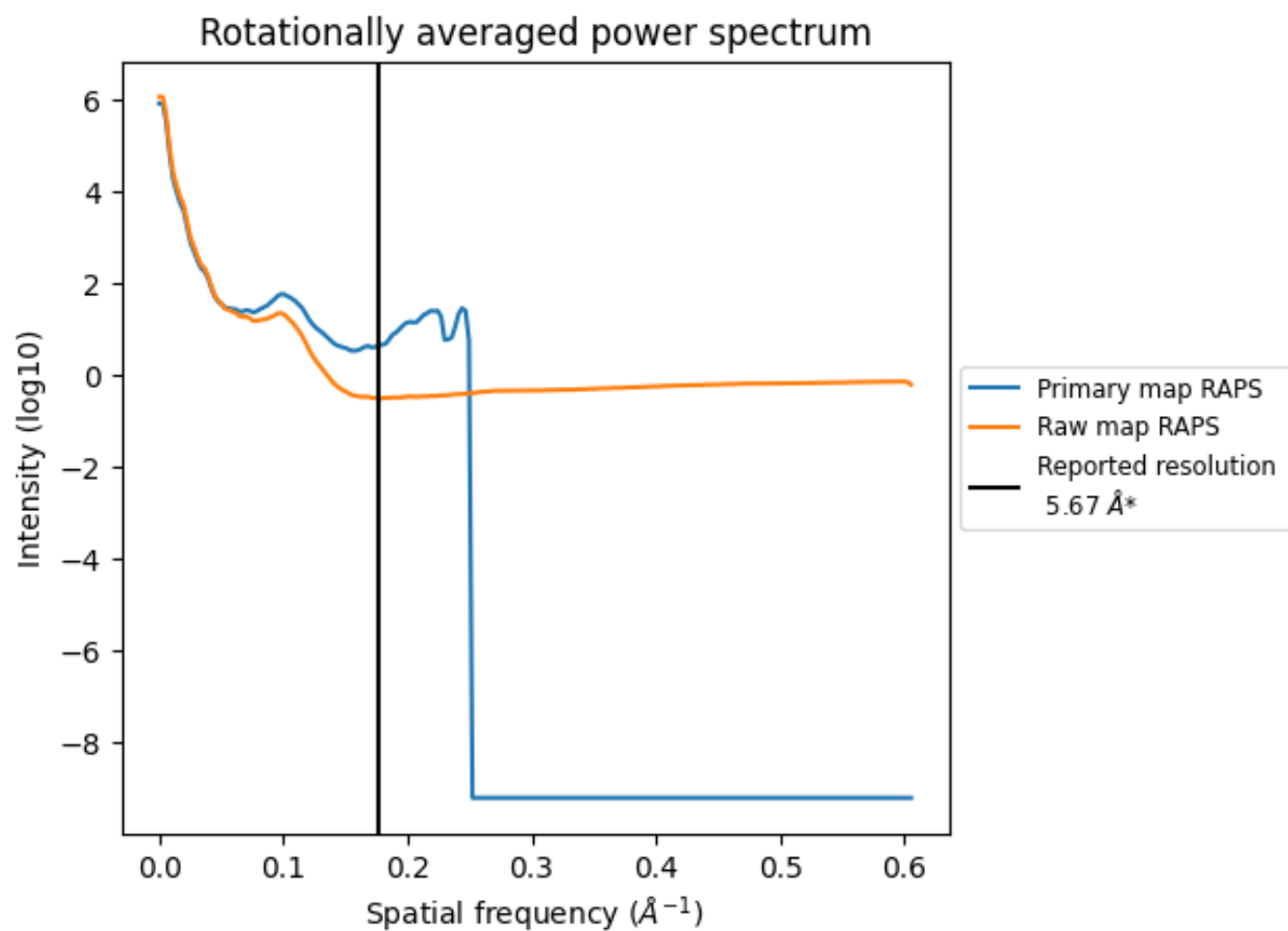
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 677 nm³; this corresponds to an approximate mass of 612 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 ⓘ

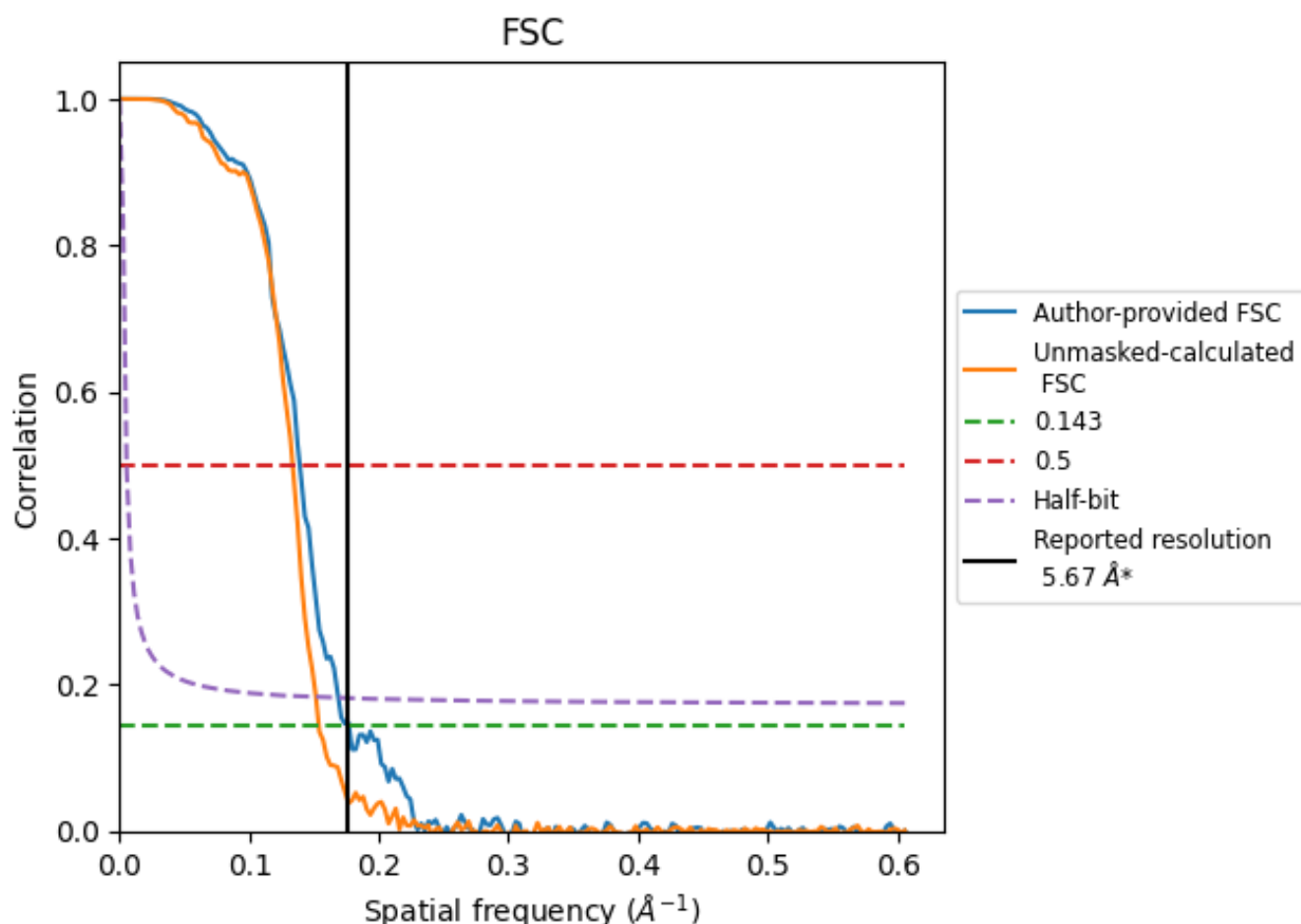


*Reported resolution corresponds to spatial frequency of 0.176 \AA^{-1}

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 0.176 Å⁻¹

8.2 Resolution estimates [i](#)

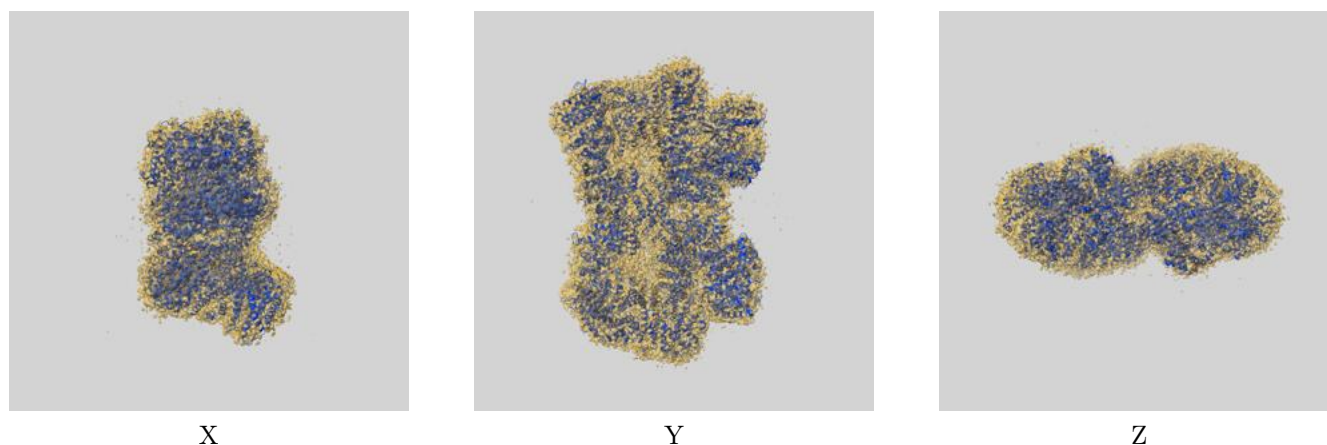
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.67	-	-
Author-provided FSC curve	5.65	7.19	5.92
Unmasked-calculated*	6.50	7.49	6.60

*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 6.50 differs from the reported value 5.67 by more than 10 %

9 Map-model fit [i](#)

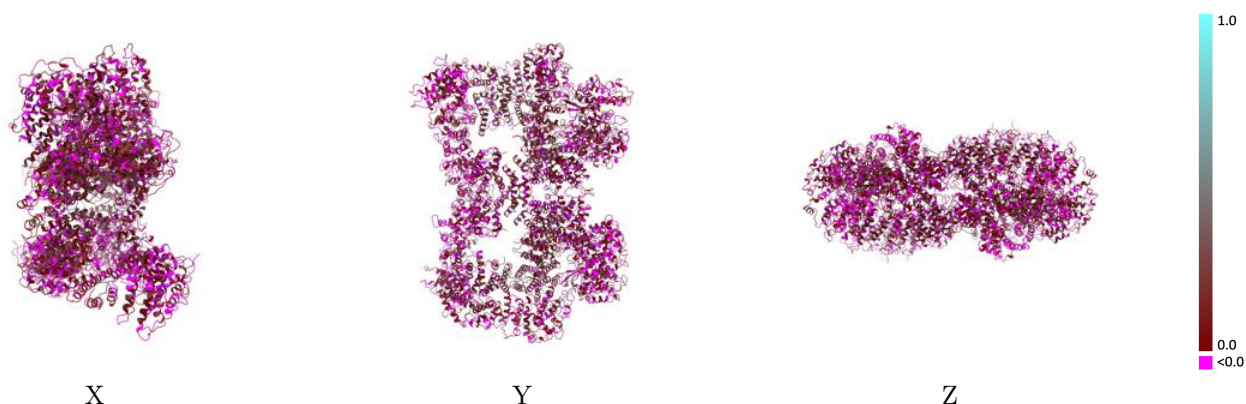
This section contains information regarding the fit between EMDB map EMD-28731 and PDB model 8EZ9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



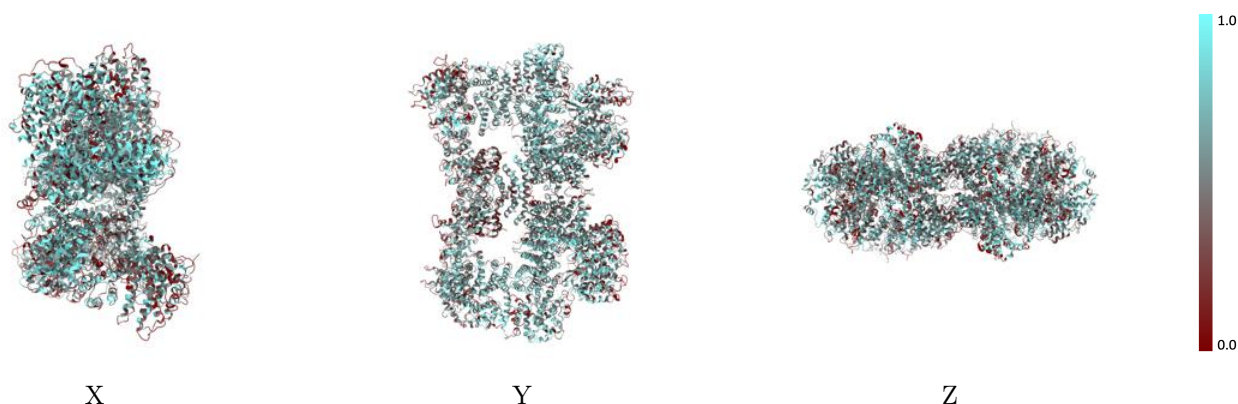
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



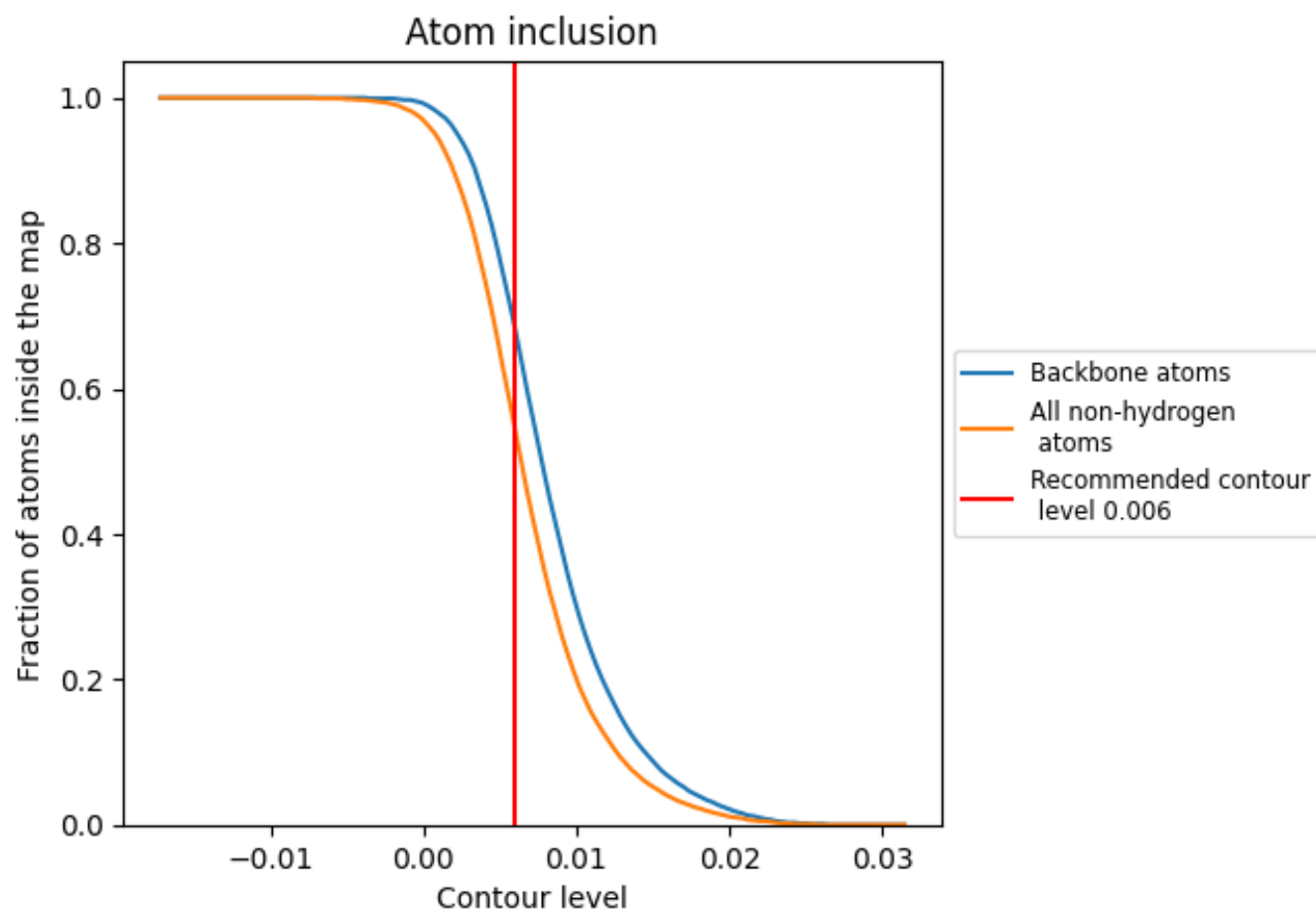
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 68% of all backbone atoms, 54% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5420	<div></div> 0.0740
C	<div></div> 0.5420	<div></div> 0.0740
L	<div></div> 0.5420	<div></div> 0.0720
Q	<div></div> 0.6040	<div></div> 0.2000
R	<div></div> 0.6240	<div></div> 0.1960

