



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:26 AM UTC

PDB ID : 8R2D / pdb_00008r2d
EMDB ID : EMD-18839
Title : Integrator cleavage module assembly intermediate
Authors : Sabath, K.; Qiu, C.; Jonas, S.
Deposited on : 2023-11-03
Resolution : 3.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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:

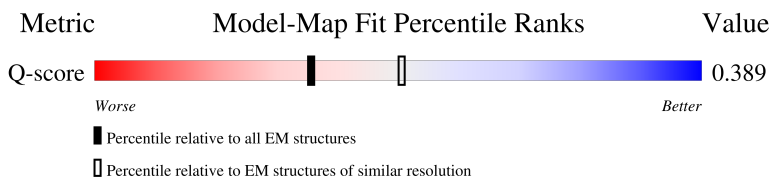
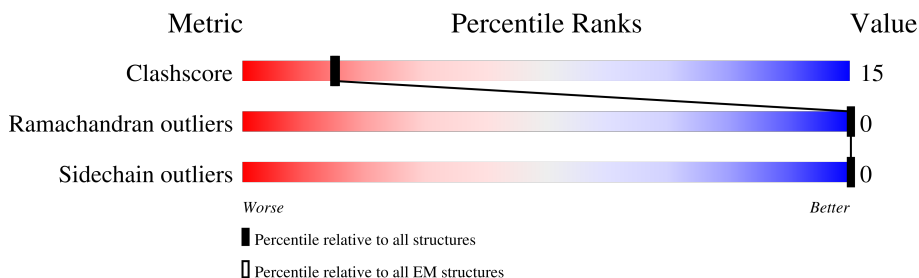
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.90 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	8855 (3.40 - 4.40)

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	827	 7% 61% 26% 13%
2	B	658	 49% 25% 27%
3	C	612	 49% 21% 30%
4	D	973	 41% 44% 29% 27%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18276 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 BRCA1-associated ATM activator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	718	Total	C	N	O	S	0	0
			5468	3482	938	1013	35		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q6PJG6
A	-4	PRO	-	expression tag	UNP Q6PJG6
A	-3	SER	-	expression tag	UNP Q6PJG6
A	-2	GLN	-	expression tag	UNP Q6PJG6
A	-1	SER	-	expression tag	UNP Q6PJG6
A	0	ASN	-	expression tag	UNP Q6PJG6

- Molecule 2 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	483	Total	C	N	O	S	0	0
			3786	2438	615	704	29		

- Molecule 3 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	429	Total	C	N	O	S	0	0
			3381	2166	576	608	31		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	GLY	-	expression tag	UNP Q5TA45
C	-10	PRO	-	expression tag	UNP Q5TA45
C	-9	SER	-	expression tag	UNP Q5TA45
C	-8	ASP	-	expression tag	UNP Q5TA45
C	-7	PRO	-	expression tag	UNP Q5TA45

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP Q5TA45
C	-5	PRO	-	expression tag	UNP Q5TA45
C	-4	LYS	-	expression tag	UNP Q5TA45
C	-3	ARG	-	expression tag	UNP Q5TA45
C	-2	ALA	-	expression tag	UNP Q5TA45
C	-1	GLU	-	expression tag	UNP Q5TA45
C	0	PHE	-	expression tag	UNP Q5TA45

- Molecule 4 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	712	Total	C	N	O	S	0	0
			5639	3590	965	1052	32		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLY	-	expression tag	UNP Q96HW7
D	-8	PRO	-	expression tag	UNP Q96HW7
D	-7	SER	-	expression tag	UNP Q96HW7
D	-6	ASP	-	expression tag	UNP Q96HW7
D	-5	PRO	-	expression tag	UNP Q96HW7
D	-4	GLY	-	expression tag	UNP Q96HW7
D	-3	PRO	-	expression tag	UNP Q96HW7
D	-2	LYS	-	expression tag	UNP Q96HW7
D	-1	ARG	-	expression tag	UNP Q96HW7
D	0	ALA	-	expression tag	UNP Q96HW7

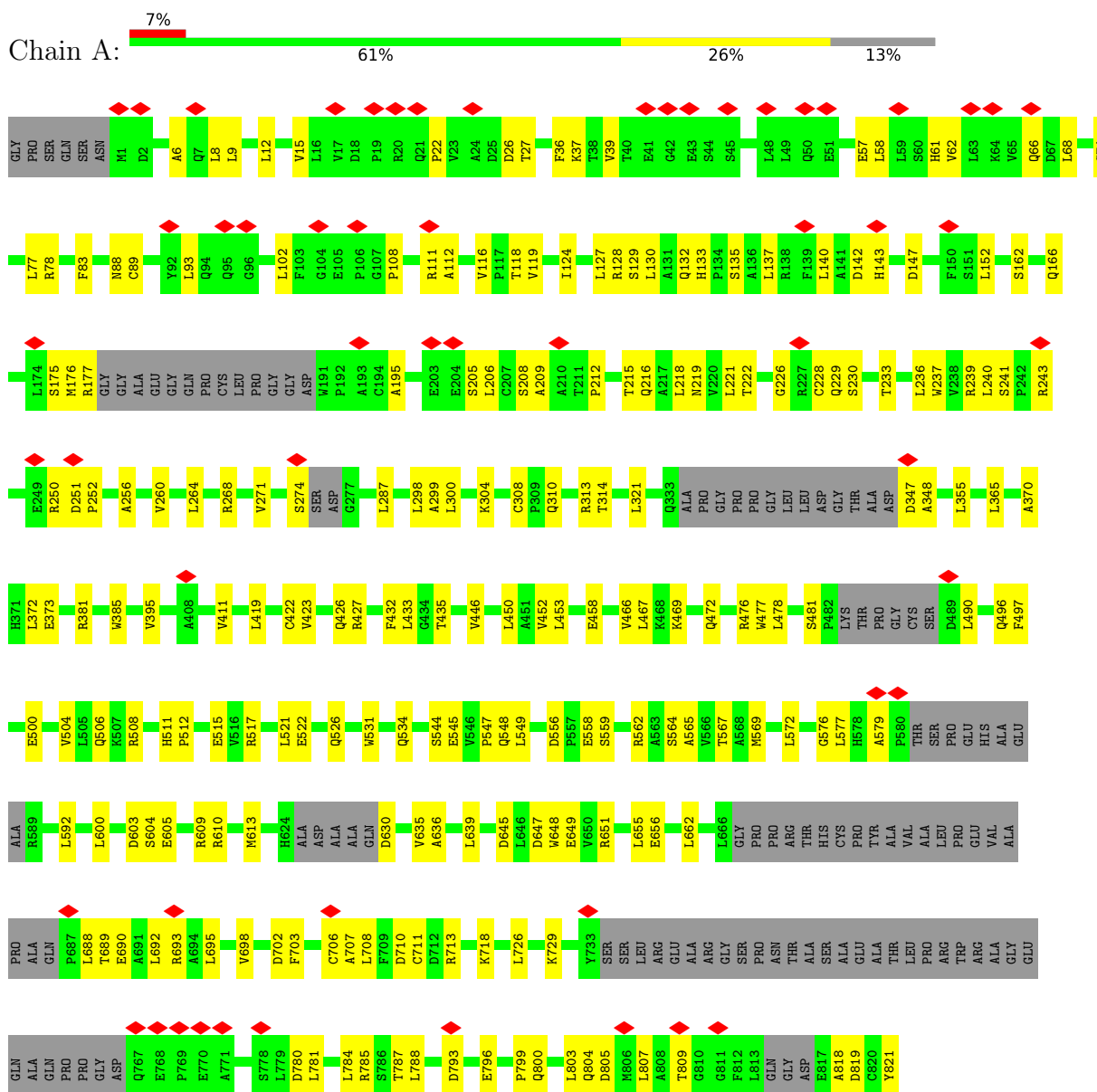
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Zn	0
			2	2	

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.

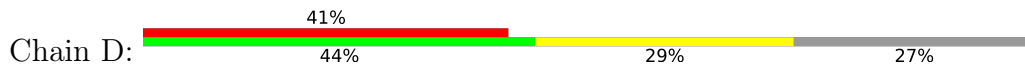
- Molecule 1: BRCA1-associated ATM activator 1



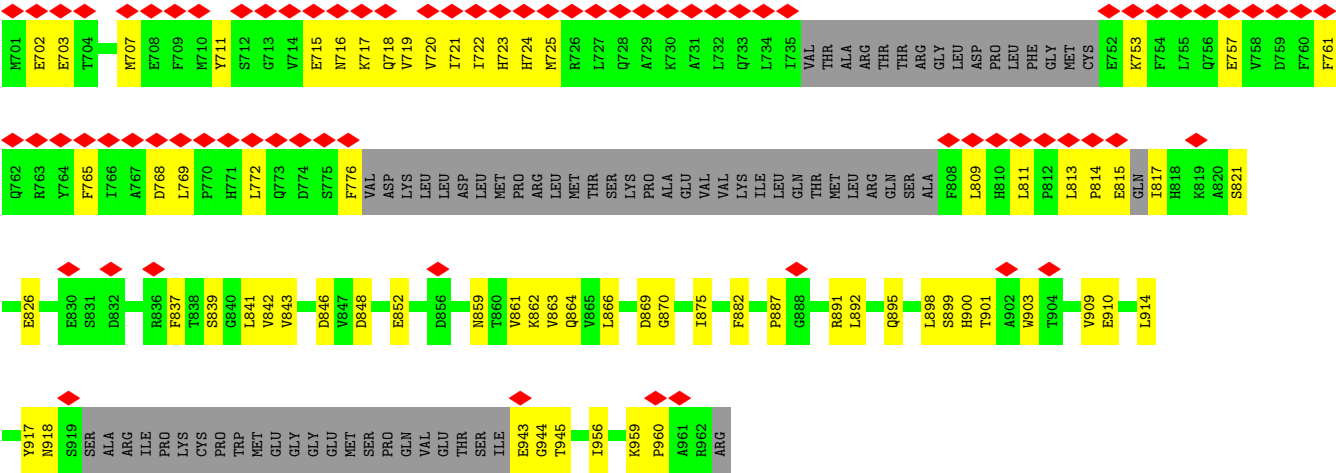
- Molecule 2: Integrator complex subunit 9



- Molecule 4: Integrator complex subunit 4



R641	D642	L643	Q644	P645	L646	G647	E648	L649	Q650	S651	E652	L653	G654	A655	S656	L657	P658	D659	I660	A661	T662	Y663	L664	R665	C666	G667	L668	L669	L670	L671	K672	A673	L674	G675	L676	L677	L678	L679	L680	
S581	H582	L583	V584	P585	A586	L587	H588	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	G547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L449	D450	T451	V452	L453	A454	V455	L456	E457	D458	H459	S460	R461	D462	T463	R464	H468	F469	L470		N475	V476	S477	I478	K479	F480	A481	G482	V483	L484	L485	L486	F487	E488	A489	L490	L491	L492	L493	L494	
L521	V522	P523	E524	L525	A526	S527	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	G547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
S581	H582	L583	V584	P585	A586	L587	H588	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M539	D540	D541	P542	I543	A544	T545	A546	G547	L548	Q549	L550	F551	L552	L553	A554	A555	L556	L557	L558
L631	D632	L633	Q634	P635	L636	G637	E638	L639	Q640	S641	E642	L643	G644	A645	S646	L647	P648	D649	I650	A651	T652	Y653	L654	R655	C656	G657	L658	L659	L660	L661	K662	A663	L664	G665	L666	L667	L668	L669	L670	
S631	H632	L633	V634	P635	A636	L637	H638	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M639	D640	D641	P642	I643	A644	T645	A646	G647	L648	Q649	L650	F651	L652	L653	A654	A655	L656	L657	L658
L721	V722	P723	E724	L725	A726	S727	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M739	D740	D741	P742	I743	A744	T745	A746	G747	L748	Q749	L750	F751	L752	L753	A754	A755	L756	L757	L758
S781	H782	L783	V784	P785	A786	L787	H788	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M789	D790	D791	P792	I793	A794	T795	A796	G797	L798	Q799	L800	F801	L802	L803	A804	A805	L806	L807	L808
L821	V822	P823	E824	L825	A826	S827	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M829	D830	D831	P832	I833	A834	T835	A836	G837	L838	Q839	L840	F841	L842	L843	A844	A845	L846	L847	L848
S881	H882	L883	V884	P885	A886	L887	H888	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M889	D890	D891	P892	I893	A894	T895	A896	G897	L898	Q899	L900	F901	L902	L903	A904	A905	L906	L907	L908
L921	V922	P923	E924	L925	A926	S927	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M929	D930	D931	P932	I933	A934	T935	A936	G937	L938	Q939	L940	F941	L942	L943	A944	A945	L946	L947	L948
S981	H982	L983	V984	P985	A986	L987	H988	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M989	D990	D991	P992	I993	A994	T995	A996	G997	L998	Q999	L1000	F1001	L1002	L1003	A1004	A1005	L1006	L1007	L1008
L1021	V1022	P1023	E1024	L1025	A1026	S1027	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1029	D1030	D1031	P1032	I1033	A1034	T1035	A1036	G1037	L1038	Q1039	L1040	F1041	L1042	L1043	A1044	A1045	L1046	L1047	L1048
S1081	H1082	L1083	V1084	P1085	A1086	L1087	H1088	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1089	D1090	D1091	P1092	I1093	A1094	T1095	A1096	G1097	L1098	Q1099	L1100	F1101	L1102	L1103	A1104	A1105	L1106	L1107	L1108
L1121	V1122	P1123	E1124	L1125	A1126	S1127	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1129	D1130	D1131	P1132	I1133	A1134	T1135	A1136	G1137	L1138	Q1139	L1140	F1141	L1142	L1143	A1144	A1145	L1146	L1147	L1148
S1181	H1182	L1183	V1184	P1185	A1186	L1187	H1188	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1189	D1190	D1191	P1192	I1193	A1194	T1195	A1196	G1197	L1198	Q1199	L1200	F1201	L1202	L1203	A1204	A1205	L1206	L1207	L1208
L1221	V1222	P1223	E1224	L1225	A1226	S1227	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1229	D1230	D1231	P1232	I1233	A1234	T1235	A1236	G1237	L1238	Q1239	L1240	F1241	L1242	L1243	A1244	A1245	L1246	L1247	L1248
S1281	H1282	L1283	V1284	P1285	A1286	L1287	H1288	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1289	D1290	D1291	P1292	I1293	A1294	T1295	A1296	G1297	L1298	Q1299	L1300	F1301	L1302	L1303	A1304	A1305	L1306	L1307	L1308
S1341	H1342	L1343	V1344	P1345	A1346	L1347	H1348	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1349	D1350	D1351	P1352	I1353	A1354	T1355	A1356	G1357	L1358	Q1359	L1360	F1361	L1362	L1363	A1364	A1365	L1366	L1367	L1368
L1381	V1382	P1383	E1384	L1385	A1386	S1387	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1389	D1390	D1391	P1392	I1393	A1394	T1395	A1396	G1397	L1398	Q1399	L1400	F1401	L1402	L1403	A1404	A1405	L1406	L1407	L1408
S1441	H1442	L1443	V1444	P1445	A1446	L1447	H1448	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1449	D1450	D1451	P1452	I1453	A1454	T1455	A1456	G1457	L1458	Q1459	L1460	F1461	L1462	L1463	A1464	A1465	L1466	L1467	L1468
L1481	V1482	P1483	E1484	L1485	A1486	S1487	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1489	D1490	D1491	P1492	I1493	A1494	T1495	A1496	G1497	L1498	Q1499	L1500	F1501	L1502	L1503	A1504	A1505	L1506	L1507	L1508
S1541	H1542	L1543	V1544	P1545	A1546	L1547	H1548	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1549	D1550	D1551	P1552	I1553	A1554	T1555	A1556	G1557	L1558	Q1559	L1560	F1561	L1562	L1563	A1564	A1565	L1566	L1567	L1568
L1581	V1582	P1583	E1584	L1585	A1586	S1587	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1589	D1590	D1591	P1592	I1593	A1594	T1595	A1596	G1597	L1598	Q1599	L1600	F1601	L1602	L1603	A1604	A1605	L1606	L1607	L1608
S1641	H1642	L1643	V1644	P1645	A1646	L1647	H1648	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1649	D1650	D1651	P1652	I1653	A1654	T1655	A1656	G1657	L1658	Q1659	L1660	F1661	L1662	L1663	A1664	A1665	L1666	L1667	L1668
L1681	V1682	P1683	E1684	L1685	A1686	S1687	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1689	D1690	D1691	P1692	I1693	A1694	T1695	A1696	G1697	L1698	Q1699	L1700	F1701	L1702	L1703	A1704	A1705	L1706	L1707	L1708
S1741	H1742	L1743	V1744	P1745	A1746	L1747	H1748	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1749	D1750	D1751	P1752	I1753	A1754	T1755	A1756	G1757	L1758	Q1759	L1760	F1761	L1762	L1763	A1764	A1765	L1766	L1767	L1768
L1781	V1782	P1783	E1784	L1785	A1786	S1787	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1789	D1790	D1791	P1792	I1793	A1794	T1795	A1796	G1797	L1798	Q1799	L1800	F1801	L1802	L1803	A1804	A1805	L1806	L1807	L1808
S1841	H1842	L1843	V1844	P1845	A1846	L1847	H1848	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1849	D1850	D1851	P1852	I1853	A1854	T1855	A1856	G1857	L1858	Q1859	L1860	F1861	L1862	L1863	A1864	A1865	L1866	L1867	L1868
L1881	V1882	P1883	E1884	L1885	A1886	S1887	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1889	D1890	D1891	P1892	I1893	A1894	T1895	A1896	G1897	L1898	Q1899	L1900	F1901	L1902	L1903	A1904	A1905	L1906	L1907	L1908
S1941	H1942	L1943	V1944	P1945	A1946	L1947	H1948	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1949	D1950	D1951	P1952	I1953	A1954	T1955	A1956	G1957	L1958	Q1959	L1960	F1961	L1962	L1963	A1964	A1965	L1966	L1967	L1968
L1981	V1982	P1983	E1984	L1985	A1986	S1987	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M1989	D1990	D1991	P1992	I1993	A1994	T1995	A1996	G1997	L1998	Q1999	L2000	F2001	L2002	L2003	A2004	A2005	L2006	L2007	L2008
S2041	H2042	L2043	V2044	P2045	A2046	L2047	H2048	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M2049	D2050	D2051	P2052	I2053	A2054	T2055	A2056	G2057	L2058	Q2059	L2060	F2061	L2062	L2063	A2064	A2065	L2066	L2067	L2068
L2081	V2082	P2083	E2084	L2085	A2086	S2087	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M2089	D2090	D2091	P2092	I2093	A2094	T2095	A2096	G2097	L2098	Q2099	L2100	F2101	L2102	L2103	A2104	A2105	L2106	L2107	L2108
S2141	H2142	L2143	V2144	P2145	A2146	L2147	H2148	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M2149	D2150	D2151	P2152	I2153	A2154	T2155	A2156	G2157	L2158	Q2159	L2160	F2161	L2162	L2163	A2164	A2165	L2166	L2167	L2168
L2181	V2182	P2183	E2184	L2185	A2186	S2187	THR	HIS	PRO	HIS	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M2189	D2190	D2191	P2192	I2193	A2194	T2195	A2196	G2197	L2198	Q2199	L2200	F2201	L2202	L2203	A2204	A2205	L2206	L2207	L2208
S2241	H2242	L2243	V2244	P2245	A2246	L2247	H2248	LEU	HIS	PRO	PHE	PHE	ASP	LEU	VAL	SER	SER	ALA	VAL	SER	M2249	D2250	D2251	P2252	I2253	A2254	T2255	A2256	G2257	L2258	Q2259	L2260	F2261	L2262						



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97185	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 ($e^-/\text{\AA}^2$)	59.5	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.118	Depositor
Minimum map value	-1.934	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.324	Depositor
Map size (Å)	298.08, 298.08, 298.08	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2959999, 1.2959999, 1.2959999	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	0.17	0/5578	0.38	0/7593
2	B	0.24	0/3884	0.47	0/5294
3	C	0.23	0/3457	0.49	0/4667
4	D	0.15	0/5739	0.38	0/7768
All	All	0.19	0/18658	0.42	0/25322

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 [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	5468	0	5506	143	0
2	B	3786	0	3787	112	0
3	C	3381	0	3371	102	0
4	D	5639	0	5693	199	0
5	C	2	0	0	0	0
All	All	18276	0	18357	541	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 15.

The worst 5 of 541 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:B:44:VAL:HG11	4:D:899:SER:HB2	1.55	0.88
2:B:30:LEU:HB2	2:B:109:ALA:HB2	1.62	0.81
4:D:114:ALA:HA	4:D:117:ILE:HD12	1.66	0.78
4:D:917:TYR:O	4:D:943:GLU:N	2.17	0.77
4:D:568:HIS:HA	4:D:571:ARG:HD2	1.67	0.77

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	698/827 (84%)	666 (95%)	32 (5%)	0	100	100
2	B	479/658 (73%)	427 (89%)	52 (11%)	0	100	100
3	C	423/612 (69%)	371 (88%)	52 (12%)	0	100	100
4	D	690/973 (71%)	665 (96%)	25 (4%)	0	100	100
All	All	2290/3070 (75%)	2129 (93%)	161 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	600/677 (89%)	600 (100%)	0	100	100
2	B	438/600 (73%)	438 (100%)	0	100	100
3	C	363/529 (69%)	363 (100%)	0	100	100
4	D	629/852 (74%)	629 (100%)	0	100	100
All	All	2030/2658 (76%)	2030 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	553	ASN
4	D	568	HIS
4	D	724	HIS
2	B	465	GLN
2	B	389	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are 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.

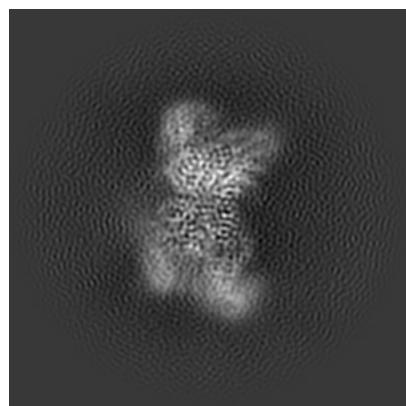
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18839. These allow visual inspection of the internal detail of the map and identification of artifacts.

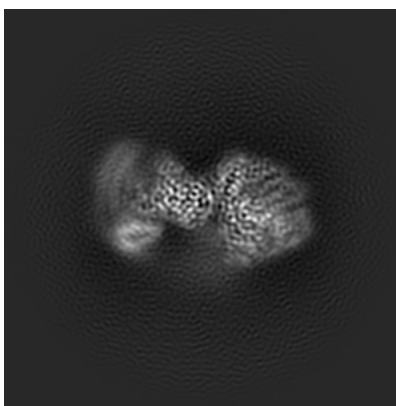
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

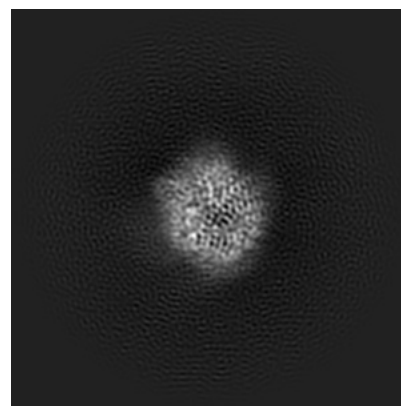
6.1.1 Primary map



X

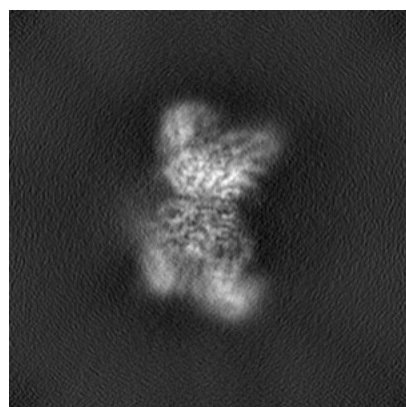


Y

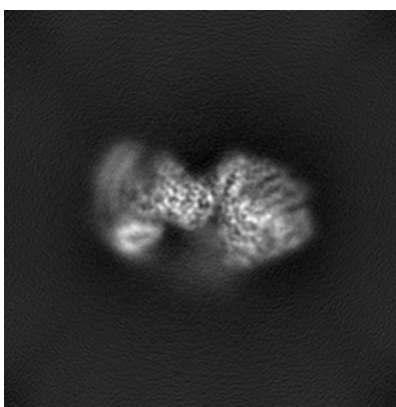


Z

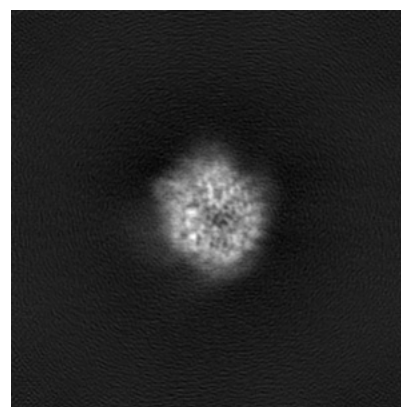
6.1.2 Raw map



X



Y

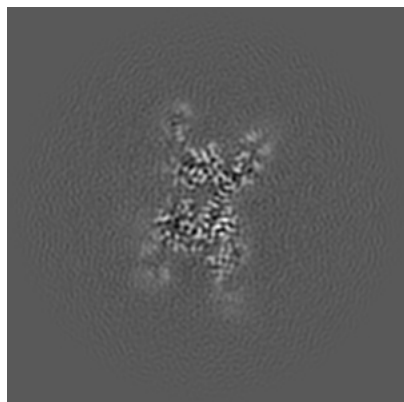


Z

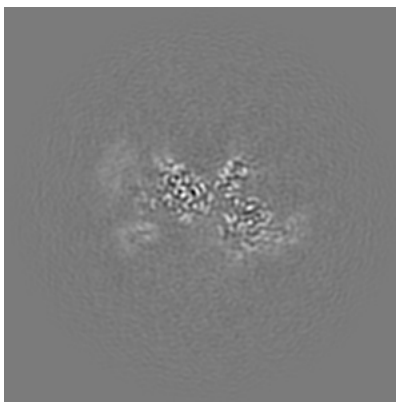
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

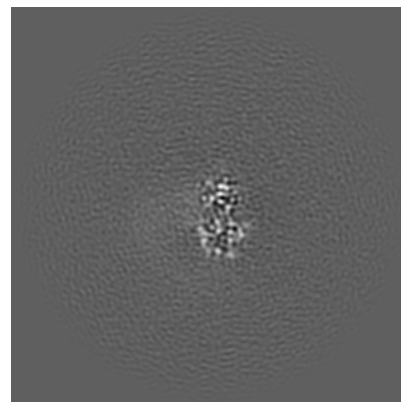
6.2.1 Primary map



X Index: 115

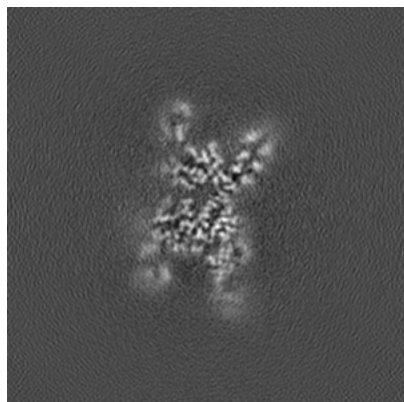


Y Index: 115

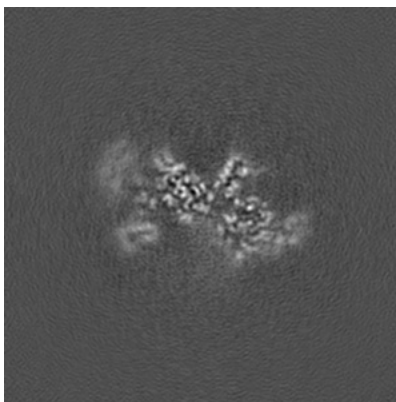


Z Index: 115

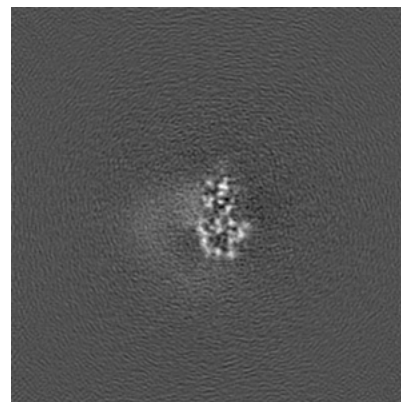
6.2.2 Raw map



X Index: 115



Y Index: 115

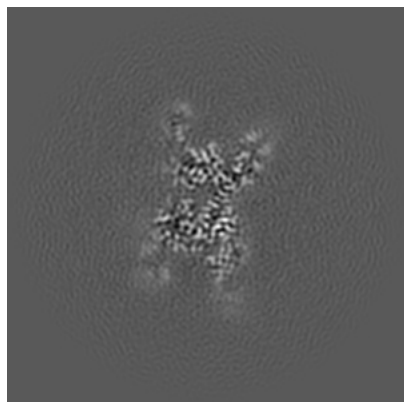


Z Index: 115

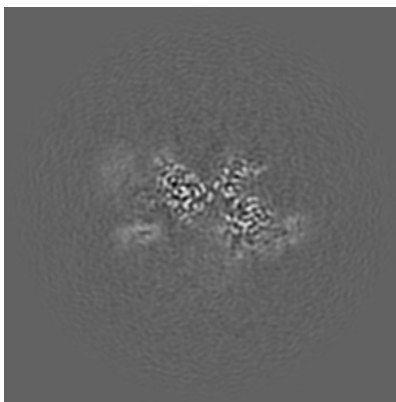
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

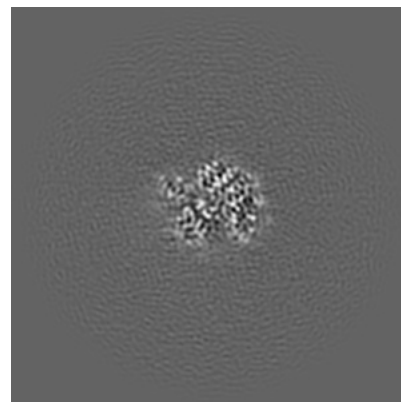
6.3.1 Primary map



X Index: 115

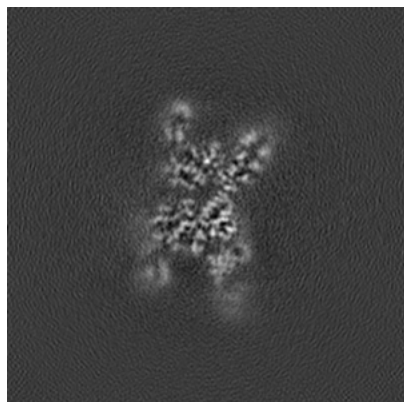


Y Index: 114

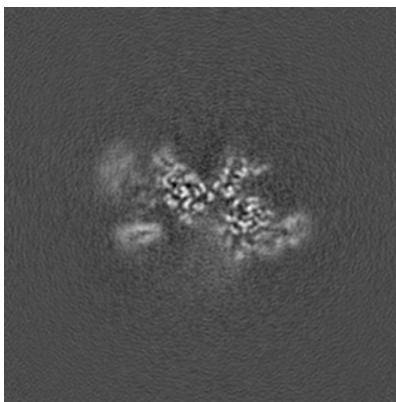


Z Index: 132

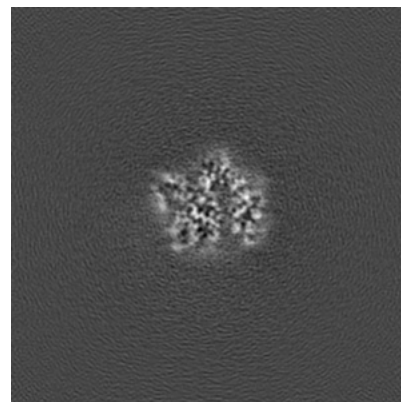
6.3.2 Raw map



X Index: 114



Y Index: 114

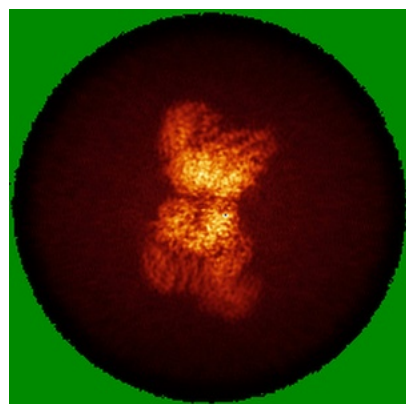


Z Index: 135

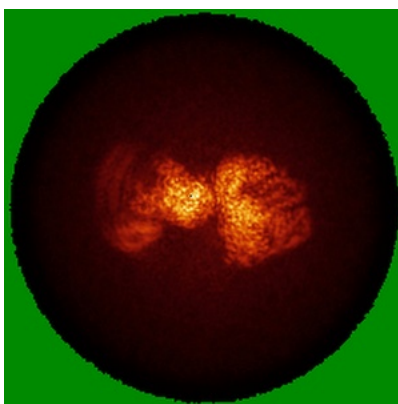
The images above show the largest variance slices of the map in three orthogonal directions.

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

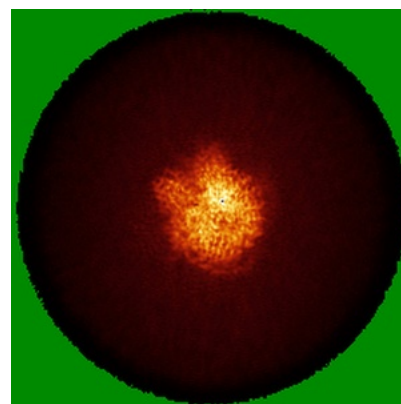
6.4.1 Primary map



X

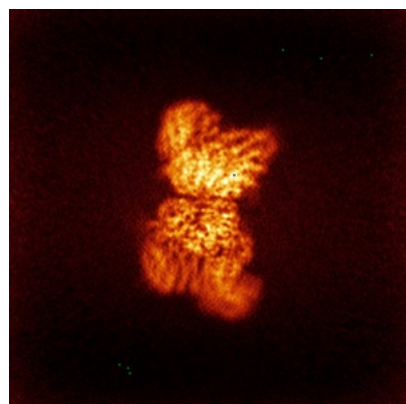


Y

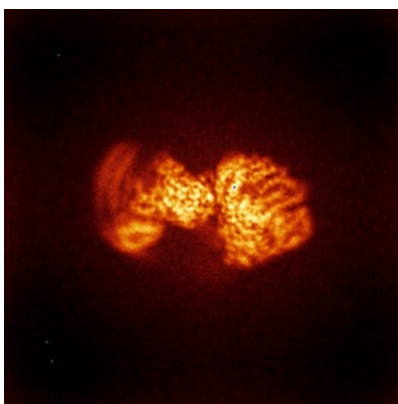


Z

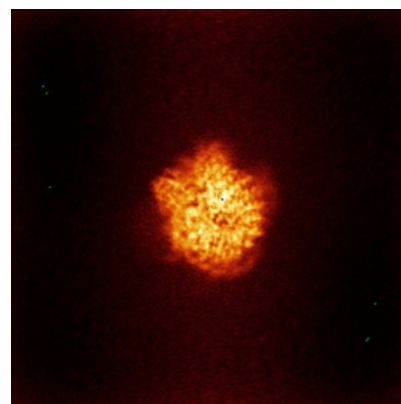
6.4.2 Raw map



X



Y

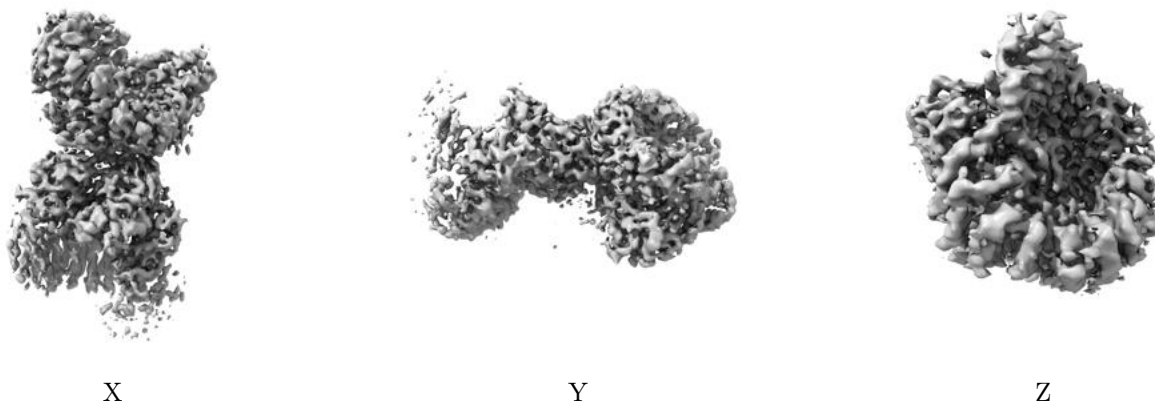


Z

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.

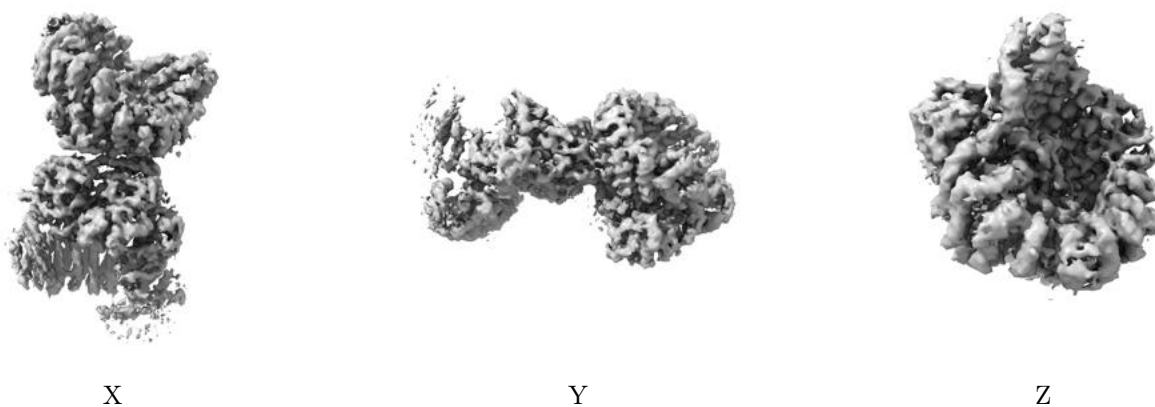
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.324. 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.

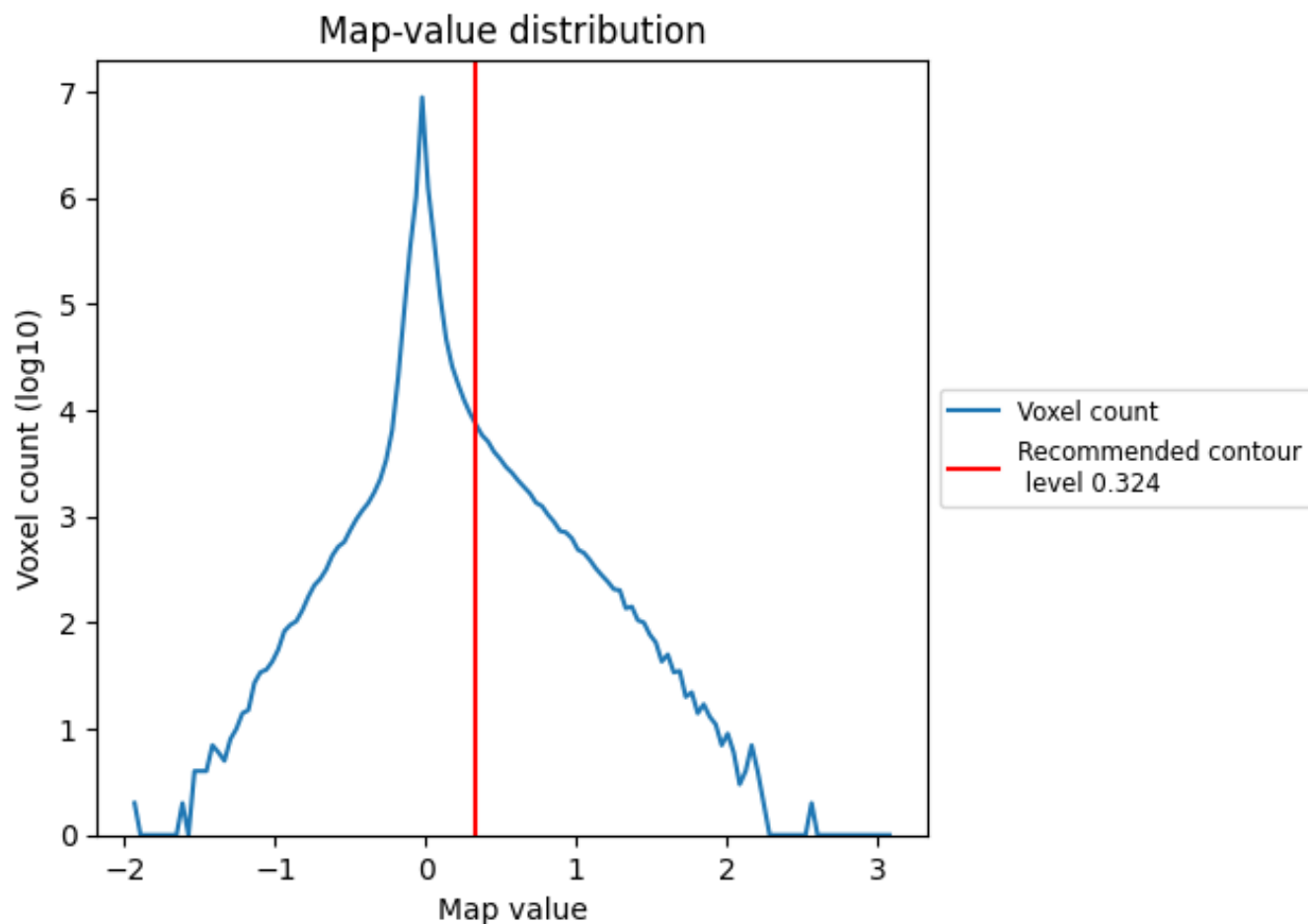
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

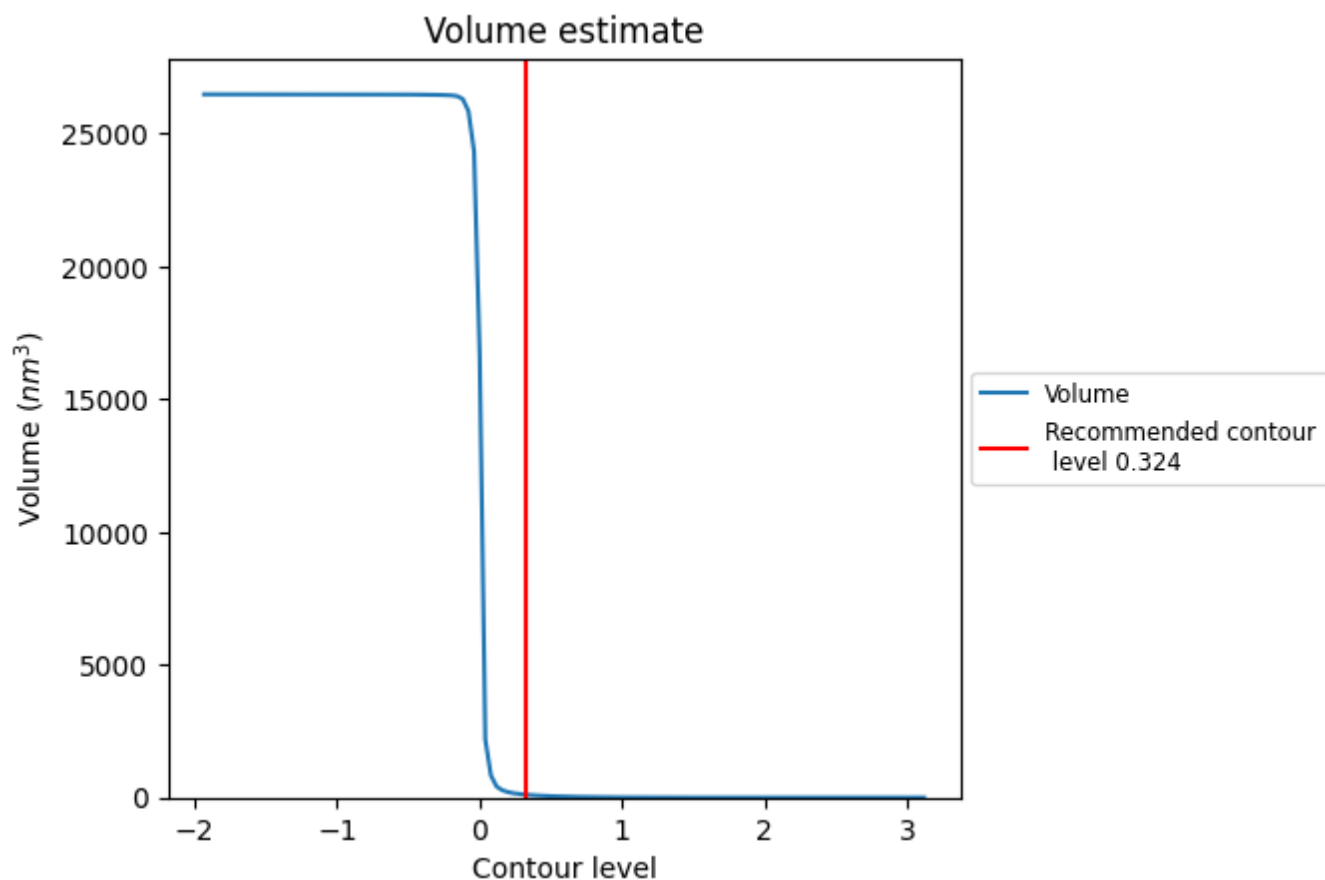
This section contains the results of statistical analysis of the map.

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.

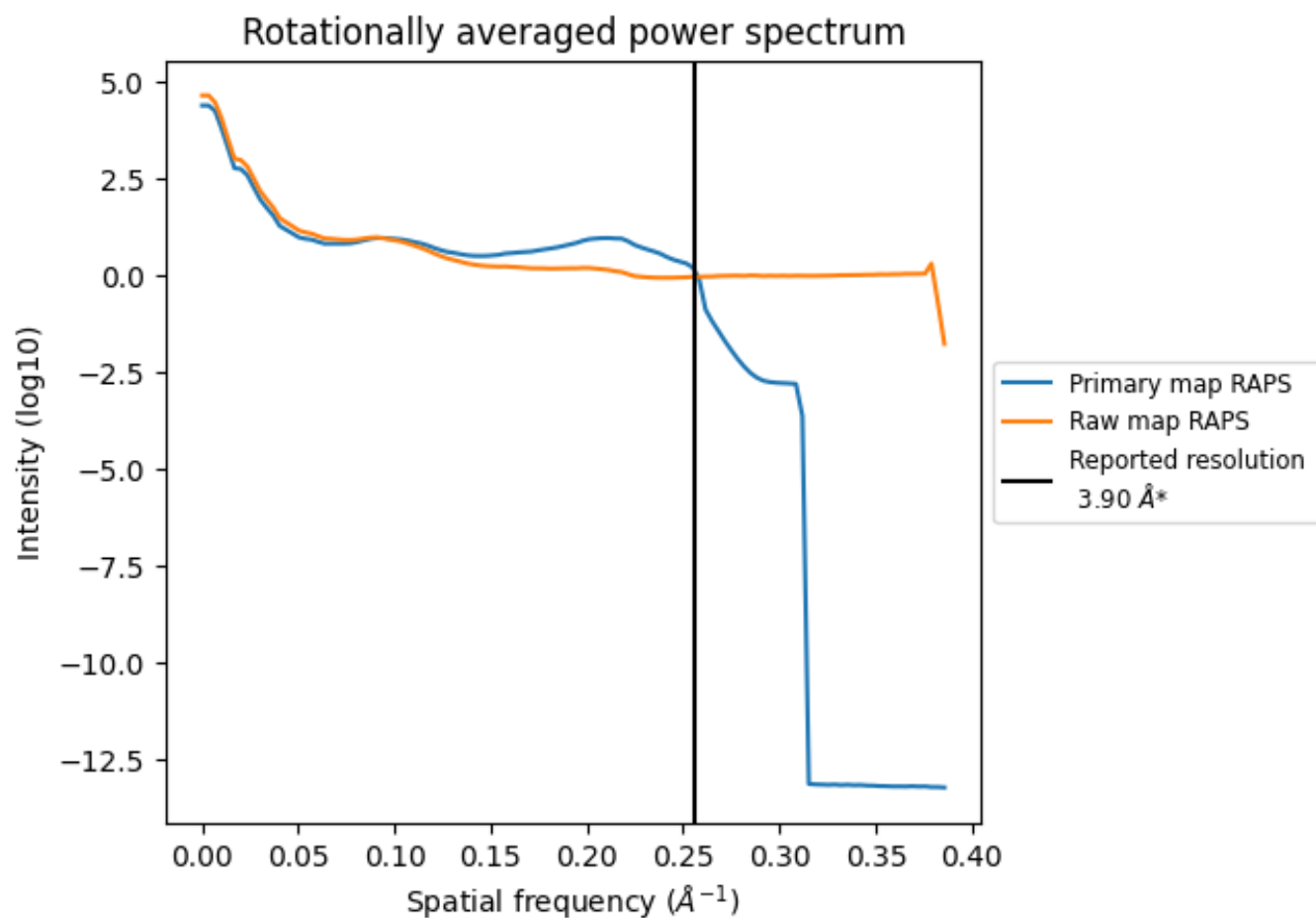
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 96 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 ⓘ

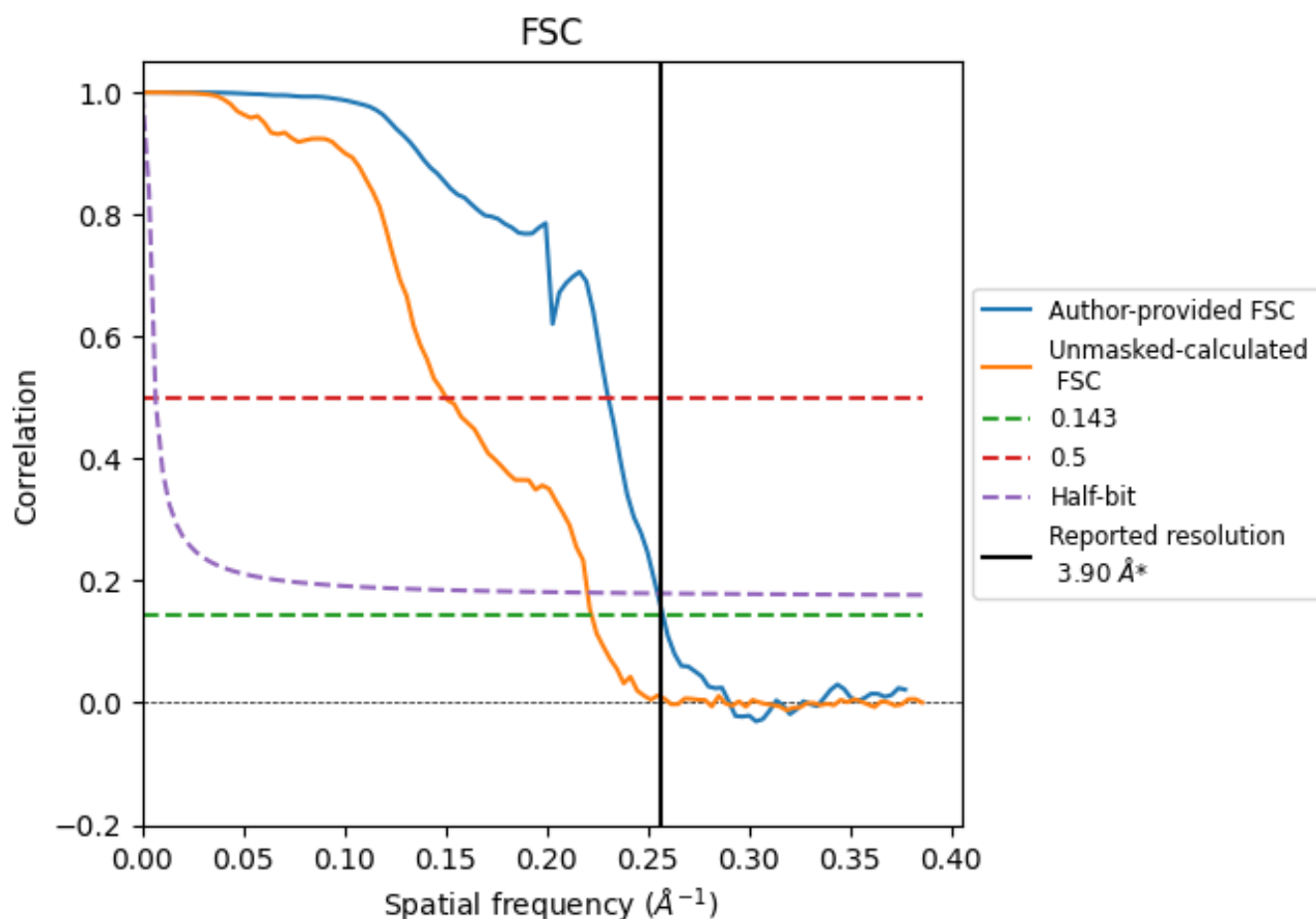


*Reported resolution corresponds to spatial frequency of $0.256 \text{ \AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

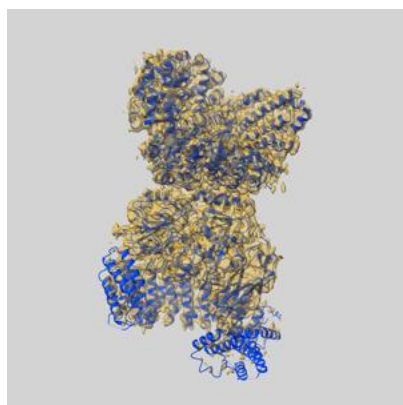
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.88	4.34	3.92
Unmasked-calculated*	4.50	6.65	4.54

*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 4.50 differs from the reported value 3.9 by more than 10 %

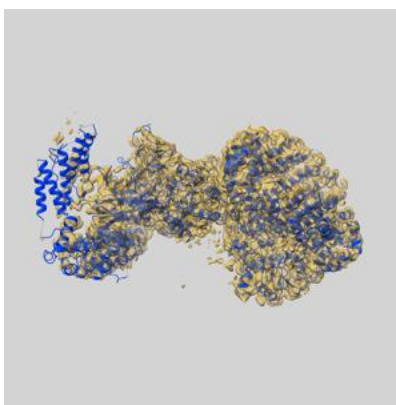
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18839 and PDB model 8R2D. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

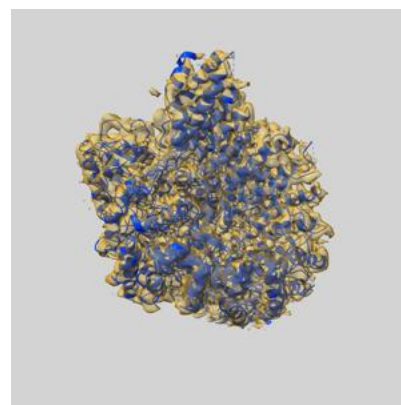
9.1 Map-model overlay [i](#)



X



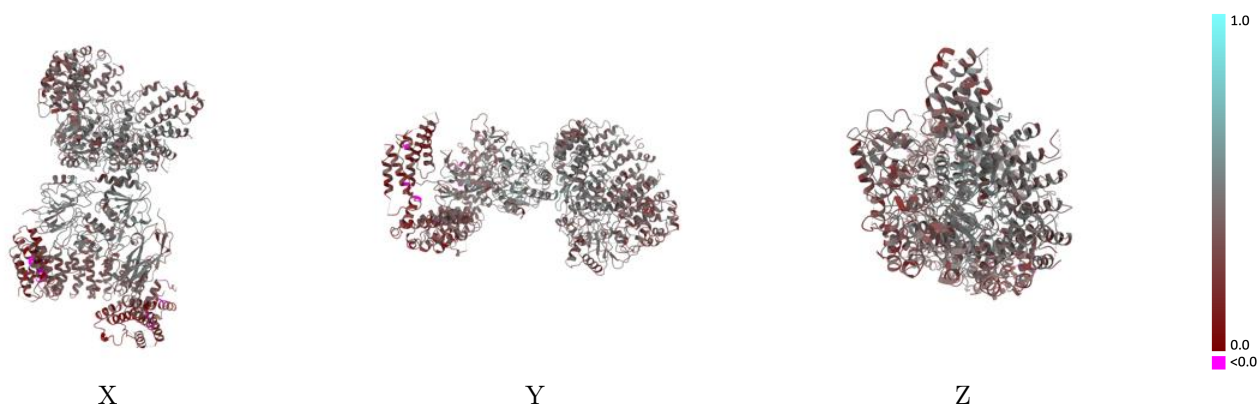
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.324 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](#)

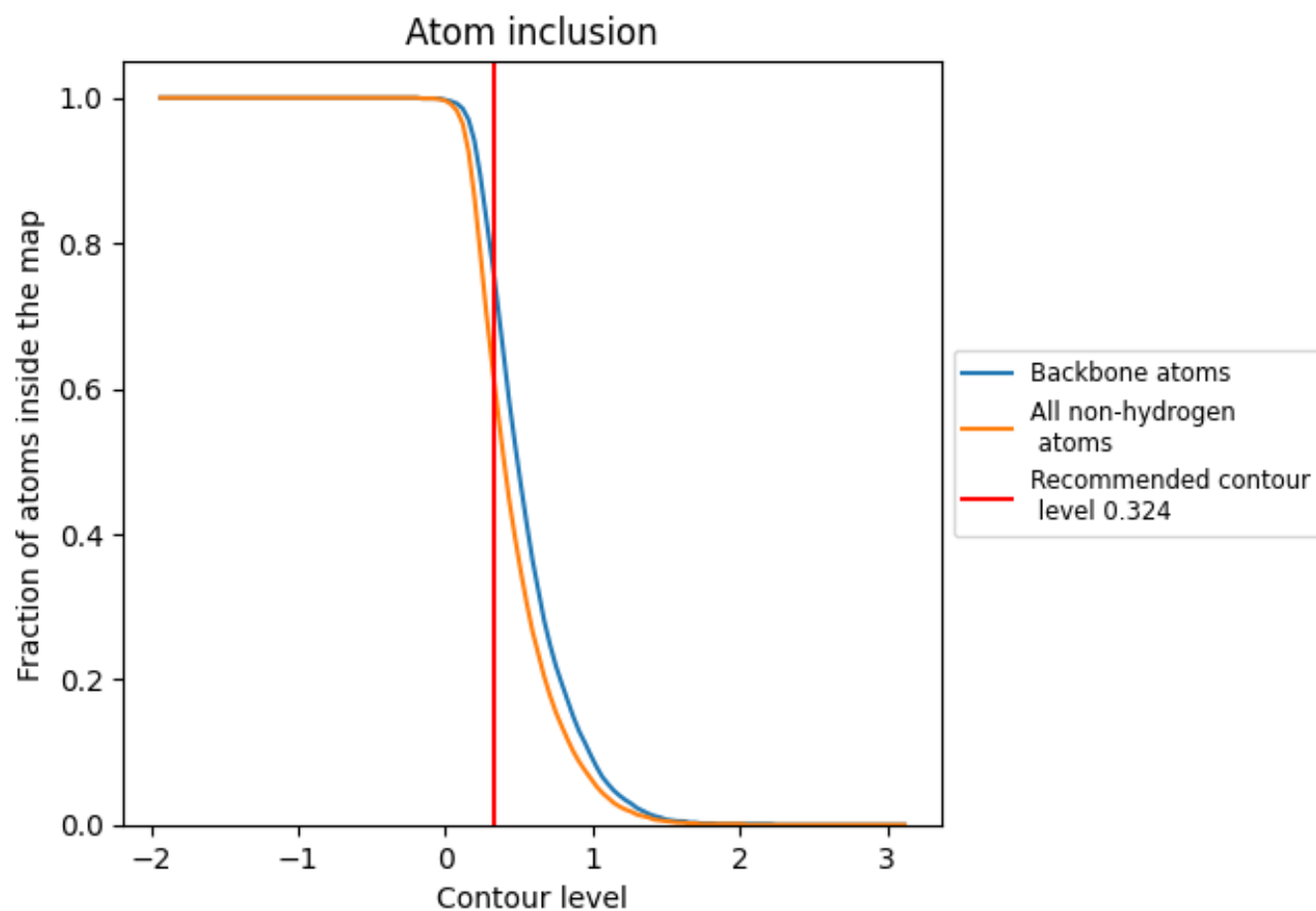


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 62% 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 (0.324) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.3890
A	0.7220	0.4090
B	0.7720	0.4570
C	0.7300	0.4260
D	0.3590	0.3010

