



wwPDB EM Validation Summary Report ⓘ

Apr 22, 2024 – 07:57 pm BST

PDB ID : 6ZH4
EMDB ID : EMD-11213
Title : Cryo-EM structure of DNA-PKcs (State 3)
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2020-06-20
Resolution : 3.62 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

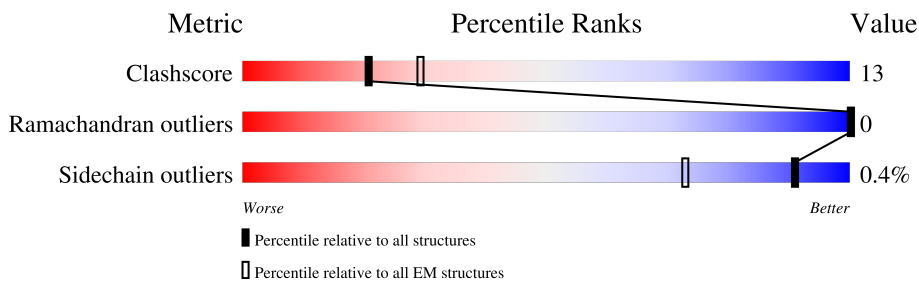
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4156	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29352 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.

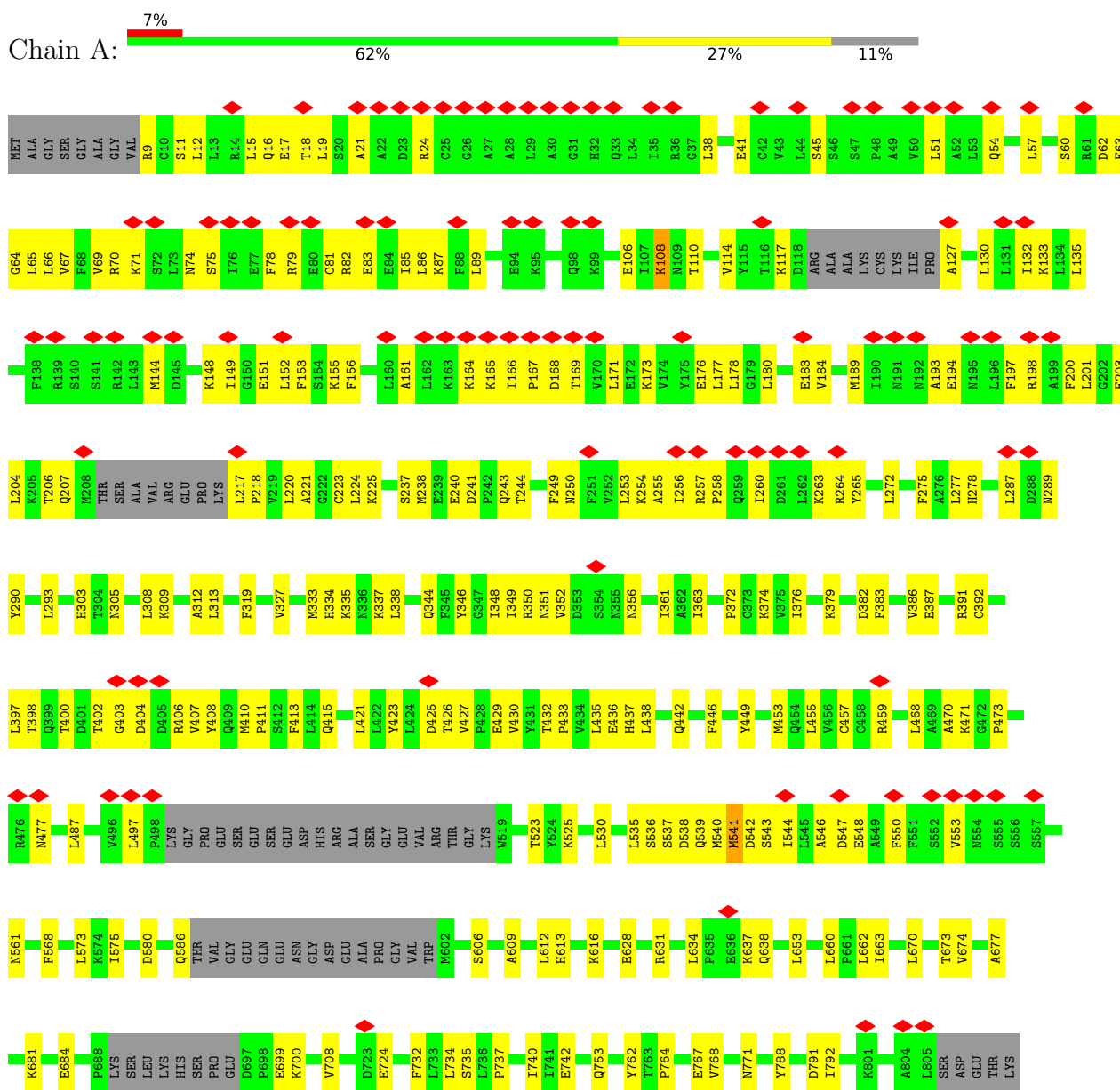
- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3698	29352	18827	4960	5372	193	0	0

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: DNA-dependent protein kinase catalytic subunit,DNA-PKCs



PRO	ASN	K890	I1017	P1154	L1264	W1350	Q1442	T1663	Q1770	L1858	Y1945	PRO
SER	ASN	R891	P1020	A1161	E1285	T1351	L1448	S1664	Q1771	N1859	N1946	SER
TYR	TRP	P897	V1021	S1162	E1285	S1352	L1455	H1665	H1772	M1859	C1947	TYR
MET	VAL	F898	D1022	L1163	T1269	P1353	C1455	F1668	V1773	F1863	A1948	MET
SER	VAL	R899	C1032	L1166	T1275	E1354	L1458	L1674	M1774	D1864	S1950	SER
SER	ALA	E900	W1039	L1170	Q1280	G1355	H1459	L1677	L1777	T1866	S1951	LEU
LEU	LEU	R901	Q1043	K1170	Q1280	W1356	L1464	L1679	F1778	I1867	V1951	SER
SER	ARG	E916	I1044	W1171	G1283	K1357	L1467	L1679	Q1779	T1868	F1956	TYR
LEU	ARG	L917	I1044	L1172	T1284	L1358	L1468	A1880	S1780	K1869	F1956	ALA
ALA	ALA	E921	Q1047	L1178	E1285	L1359	P1469	D1881	S1781	K1870	H1957	ALA
ALA	GLN	S922	Q1048	P1179	A1286	K1360	S1470	A1881	F1782	D1878	K1970	ASP
GLY	ARG	ASP	Q1049	Q1180	S1289	C1364	K1468	G1690	R1783	D1878	M1974	SER
PHE	ARG	ARG	Q1050	T1181	L1290	M1365	L1472	Q1691	R1784	P1886	N1974	LEU
ASN	GLN	GLN	K927	F1182	L1298	M1366	S1472	Q1692	S1785	K1886	K1974	SER
LYS	VAL	T926	K1051	C1183	L1299	H1367	D1474	V1693	S1786	D1887	L1977	GLY
VAL	VAL	K927	K1061	M1184	L1475	L1368	H1475	L1694	S1787	D1888	F1978	GLU
VAL	VAL	W928	K1061	K1185	L1477	M1369	H1477	L1695	A1786	V1889	F1978	MET
LEU	LEU	E932	H1069	H1186	I1300	L1372	H1478	L1702	T1793	V1890	I1977	GLN
HIS	HIS	N937	P1070	R1202	I1301	F1384	H1483	T1703	S1800	H1891	L1981	GLN
LEU	LEU	W938	A1072	M1205	H1304	I1386	Y1488	T1704	S1803	K1892	L1982	PHE
LYS	LYS	P948	F1073	L1206	D1305	G1387	Y1492	T1705	E1803	F1805	I1982	PHE
LYS	THR	PRO	K1074	L1208	A1308	D1388	A1492	G1704	M1804	R1811	L1985	PHE
LYS	LYS	GLY	R1075	L1209	A1309	I1388	P1493	S1706	H1804	L1812	K1985	THR
ASN	ASN	GLY	F1076	K1209	E1310	G1389	G1494	G1707	L1805	L1813	E1985	THR
SER	SER	GLY	R1075	D1210	E1312	V1391	D1495	S1708	F1805	S1813	E1985	THR
SER	SER	GLY	L1080	K1213	C1312	M1392	E1496	E1708	F1805	T1814	E1985	THR
ASN	ASN	GLN	A1081	E1214	PHE	L1395	R1497	E1709	V1820	L1815	E1985	THR
GLU	ALA	GLU	F1082	E1214	GLY	T1396	E1497	V1719	V1820	L1816	E1985	THR
ALA	ALA	GLU	N1084	E1214	GLY	D1397	Q1498	V1723	D1821	L1817	E1985	THR
S847	S847	P957	N1085	E1214	GLY	D1397	C1499	M1724	D1821	L1818	E1985	THR
R854	R854	L961	Y1086	E1214	GLY	D1397	C1499	Q1725	L1827	L1819	E1985	THR
G860	G860	T965	E1088	E1214	GLY	D1397	C1499	Q1726	L1827	L1820	E1985	THR
G864	G864	L969	E1088	E1214	GLY	D1397	C1499	S1726	L1827	L1821	E1985	THR
K868	K868	L978	E1088	E1214	GLY	D1397	C1499	R1727	S1832	L1822	E1985	THR
V873	V873	D977	E1093	E1214	GLY	D1397	C1499	E1728	S1832	L1823	E1985	THR
T874	T874	Q978	E1093	E1214	GLY	D1397	C1499	F1729	A1835	L1824	E1985	THR
S875	S875	Y984	E1093	E1214	GLY	D1397	C1499	G1732	E1838	L1825	E1985	THR
D877	D877	E985	E1093	E1214	GLY	D1397	C1499	M1738	S1841	L1826	E1985	THR
S876	S876	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1827	E1985	THR
D877	D877	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1828	E1985	THR
E878	E878	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1829	E1985	THR
M879	M879	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1830	E1985	THR
M880	M880	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1831	E1985	THR
K881	K881	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1832	E1985	THR
S882	S882	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1833	E1985	THR
D887	D887	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1834	E1985	THR
R888	R888	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1835	E1985	THR
E889	E889	E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1836	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1837	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1838	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1839	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1840	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1841	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1842	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1843	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1844	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1845	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1846	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1847	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1848	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1849	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1850	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1851	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1852	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1853	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1854	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1855	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1856	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1857	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1858	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1859	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1860	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1861	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1862	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1863	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1864	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1865	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1866	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1867	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1868	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1869	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1870	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1871	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1872	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1873	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1874	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1875	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1876	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1877	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1878	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1879	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1880	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1881	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1882	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1883	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1884	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1885	E1985	THR
		E985	E1093	E1214	GLY	D1397	C1499	L1747	T1842	L1886	E1985	THR

R3380	L3298	D3068	W2993	Q2795	LYS	ASP	L2477	P2372	V2272	L2189	GLU
Q3383	L3302	Q3059	Y2930	K2806	GLY	TRP	I2480	P2373	G2273	S2174	LEU
S3386	L3307	L3062	L2933	D2821	ALA	THR	P2487	L2374	I2274	G2178	M2085
Q3390	D3308	I3065	G2934	K2822	GLY	GLY	E2488	M2379	G2278	H2183	M2086
E3393	E3309	M3069	E2935	E2829	THR	SER	S2489	V2382	A2282	H2183	R2090
E3394	N3310	I3077	S2945	K2835	ASP	THR	E2490	L2398	N2283	Y2184	H2091
E3395	N3311	L3078	E2946	L2837	LEU	PRO	D2491	E2399	D2289	M2185	E2092
A3396	V3312	L3066	K2950	Q2838	LEU	LEU	D2492	L2402	T2294	V2186	C2093
PRO	S3313	L3089	ARG	R2842	VAL	ASP	N2493	C2403	I2299	M2094	M2094
PRO	Y3315	L3089	ARG	R2843	HIS	THR	D2494	R2404	Q2296	L2100	L2100
SER	L3316	L3092	PHE	F2844	THR	THR	S2495	R2404	S2295	H2103	H2103
TRP	N3319	L3092	MET	L2844	PRO	SER	I2498	M2408	S2297	L2193	L2193
SER	I3320	K3100	ARG	N2845	GLN	GLY	L2501	T2409	E2298	L2194	L2194
CYS	L3321	I3103	ASP	T2846	THR	THR	L2506	E2410	Y2299	S2195	S2195
GLY	F3322	I3103	GLN	T2847	ASP	THR	L2506	L2411	L2303	W2196	R2106
PRO	F3323	L3121	LEU	F2848	SER	LEU	L2506	Y2412	L2303	T2197	S2107
SER	N3327	L3121	LEU	F2848	SER	GLN	L2506	L2415	M2306	P2202	L2108
ARG	I3328	K3128	LEU	F2850	ARG	THR	L2511	L2415	F2309	D2208	GLY
GLU	L3329	K3128	MET	F2854	ALA	GLN	D2512	D2419	F2309	L2211	PRO
VAL	L3341	A3134	TYR	C2857	ALA	GLY	N2514	V2420	K2313	R2214	PRO
GLN	L3341	L3135	ALA	S2862	ALA	GLY	L2517	V2421	Y2316	L2215	GLN
GLU	A3346	T3136	ARG	C2857	ARG	SER	L2521	Q2422	L2323	R2215	GLY
GLU	C3347	E3137	LYS	S2862	LEU	LEU	N2523	V2422	L2327	L2216	GLU
GLU	C3347	E3140	VAL	A2867	LEU	LEU	L2540	Q2432	L2327	M2220	ASP
ALA	E3349	L3144	ALA	L2868	GLN	TRP	L2540	R2433	R2328	F2231	VAL
SER	E3350	F3144	GLU	D2872	ARG	ARG	L2542	R2433	Y2329	F2231	P2119
ILE	I3351	K3147	GLN	Q2886	ALA	VAL	L2543	R2444	V2330	F2231	R2120
ASP	E3352	Q3148	ARG	Q2886	PRO	ALA	N2543	P2444	V2330	T2240	P2123
SER	E3353	N3150	LYS	I2890	PRO	ALA	L2543	K2445	E2332	L2241	S2124
ALA	D3354	L3151	GLY	P2902	LEU	LEU	L2547	K2445	R2333	V2242	M2125
GLU	R3357	S3152	ILE	ALA	LEU	LEU	P2547	R2452	E2333	E2243	M2126
ALA	R3357	Q3154	LYS	ALA	LEU	LEU	K2548	L2455	R2334	C2244	K2127
ALA	I3359	Q3154	SER	ALA	LEU	LEU	L2550	L2455	N2335	L2128	F2128
LEU	L3360	K3158	GLY	ALA	LEU	LEU	L2555	L2455	L2337	H2130	H2130
LEU	E3361	K3158	GLY	ALA	LEU	LEU	L2555	P2457	E2338	G2131	G2131
LEU	L3362	K3158	LEU	ALA	LEU	LEU	A2558	V2458	E2339	K2132	K2132
LEU	S3363	L3161	LYS	ALA	LEU	LEU	A2558	V2458	S2340	L2146	L2146
LEU	G3364	W3164	LYS	ALA	LEU	LEU	F2561	E2460	E2343	A2147	A2147
LEU	S3365	W3164	ARG	ALA	LEU	LEU	L2562	F2461	L2344	K2148	K2148
LEU	S3366	Y3168	VAL	ALA	LEU	LEU	L2566	H2464	L2344	L2149	L2149
LEU	S3367	P3169	ASP	ALA	LEU	LEU	T2566	P2465	L2349	W2150	W2150
LEU	R3281	P3169	GLY	ALA	LEU	LEU	S2569	S2466	L2349	I2151	I2151
LEU	R3282	M3173	LYS	ALA	LEU	LEU	S2569	S2466	Q2353	T2153	T2153
LEU	L3283	D3174	LYS	ALA	LEU	LEU	P2575	S2466	N2354	T2153	T2153
LEU	S3284	D3174	ASP	ALA	LEU	LEU	M2576	S2466	N2354	G2262	G2262
LEU	H3285	W3179	VAL	ALA	LEU	LEU	M2576	S2466	N2354	K2263	K2263
LEU	E3295	D3180	ASP	ALA	LEU	LEU	M2576	S2466	N2354	S2267	S2267
LEU	Q3296	D3181	ASN	ALA	LEU	LEU	M2576	S2466	N2354	K2268	K2268
LEU	V3297	I3182	SER	ALA	LEU	LEU	M2576	S2466	N2354	S2166	S2166
LEU	L3298	I3182	VAL	ALA	LEU	LEU	M2594	S2466	N2354	N2270	N2270
LEU	L3301	L3197	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	K3302	L3197	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3307	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	D3308	LEU	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	E3309	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	N3310	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	N3311	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	V3312	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	S3313	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	S3314	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	Y3315	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3316	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	N3319	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	I3320	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3321	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	A3322	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	F3323	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	N3327	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	I3328	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3329	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3341	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	A3346	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	C3347	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	R3348	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	A3349	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	E3350	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	I3351	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	E3352	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	E3353	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	D3354	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	R3357	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	I3359	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3360	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	E3361	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3362	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	S3363	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	G3364	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	S3365	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	S3366	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	S3367	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	E3368	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3283	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	S3284	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	H3285	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	E3295	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	Q3296	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	V3297	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3298	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3301	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	K3302	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	L3307	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	D3308	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	E3309	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	N3310	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	N3311	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	V3312	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354	S2271	S2271
LEU	S3313	PRO	THR	ALA	LEU	LEU	M2594	S2466	N2354</		

X5009	X6020	I4031	I4032	V4033	A4034	E4035	K4036	M4037	M4038	V4039	R4049	K4050	G4053	A4054	I4059	D4062	E4063	L4064	L4065	E4069	K4070	A4071	A4072	A4073	F4074	R4075	D4076	Y4077	A4081	S4084	H4087	H4088	T4089	R4090	A4091	Q4092	S4096	G4097	Q4103	V4104	L4107	M4108	D4113	R4119	E4125	M4128	R3901	A3909	L3910	M3916	D3922	R3923	M3932	D3941	H3944	A3949	L3953	P3954	V3955	P3956	E3957	L3958	M3959	R3965	N3969	L3970	M3974	K3975	I3983	M3984	L3988	R3989	R3992	S3993	D3994	V4004	W4013	K4014	E4017	K4022	G4023	G4024	G4025	S4026	W4027	I4028	Q4029	E4030	L3758	R3759	Q3760	D3761	A3780	C3781	S3782	Q3783	R3784	A3785	L3786	V3793	R3799	L3800	G3801	L3802	L3803	V3810	T3819	E3823	A3827	R3833	A3834	Y3839	L3843	K3849	Y3855	M3856	Y3859	K3860	N3863	R3864	T3867	F3871	R3874	E3875	V3878	F3879	A3880	A3886	S3674	K3675	P3676	G3677	G3678	K3681	E3682	C3683	S3684	P3685	W3686	M3687	F3690	E3693	F3694	L3695	R3696	N3697	E3698	Y3705	D3706	G3707	K3710	P3711	L3712	R3718	F3722	D3723	E3724	V3728	S3731	R3734	P3735	K3736	R3741	G3742	H3743	D3744	E3745	R3746	E3747	L3751	V3752	K3753	G3754	E3755	D3757	K3603	K3604	N3605	I3606	E3607	K3608	E3611	R3612	M3613	Y3614	L3617	K3621	A3622	P3623	F3628	R3629	R3630	K3631	T3635	F3636	G3637	K3638	E3639	F3640	D3641	K3642	H3643	K3646	G3647	G3648	S3649	K3650	L3651	L3652	R3653	M3654	K3655	S3657	D3658	F3659	N3660	D3661	I3662	T3663	M3664	M3665	L3666	L3667	M3670	N3671	K3672	D3673	L3506	D3509	Q3510	A3511	Q3515	Y3531	P3532	F3533	S3536	S3539	K3543	G3548	H3549	K3550	N3551	K3552	E3553	F3554	V3555	A3556	R3557	I3558	K3559	S3560	K3561	L3562	D3563	Q3564	L3575	D3576	Q3577	L3578	E3582	K3586	D3587	K3588	N3589	S3590	V3592	R3593	K3594	E3595	L3596	A3597	K3598	T3599	F3600	V3601	N3602
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47183	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 ($e^-/\text{\AA}^2$)	53.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	280.36002, 280.36002, 280.36002	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.652, 0.652, 0.652	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	$\# Z > 5$
1	A	0.31	0/29811	0.45	0/40307

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	29352	0	29489	783	0
All	All	29352	0	29489	783	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 13.

The worst 5 of 783 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:3628:PHE:H	1:A:3684:SER:HB3	1.42	0.85
1:A:1712:ARG:HH12	1:A:1716:GLN:HB2	1.44	0.82
1:A:3282:ARG:HE	1:A:3329:LEU:HD21	1.46	0.80
1:A:1351:THR:HG22	1:A:1353:PRO:HD2	1.61	0.80
1:A:3482:LEU:HD12	1:A:3482:LEU:O	1.81	0.80

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	3632/4156 (87%)	3357 (92%)	275 (8%)	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	3229/3671 (88%)	3215 (100%)	14 (0%)	91 96

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1738	ASN
1	A	1895	LYS
1	A	3849	LYS
1	A	3482	LEU
1	A	3552	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	303	HIS
1	A	3154	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	96.48
1	A	5016:UNK	C	6001:UNK	N	49.88

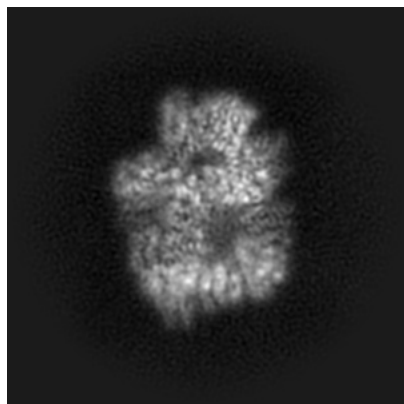
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11213. These allow visual inspection of the internal detail of the map and identification of artifacts.

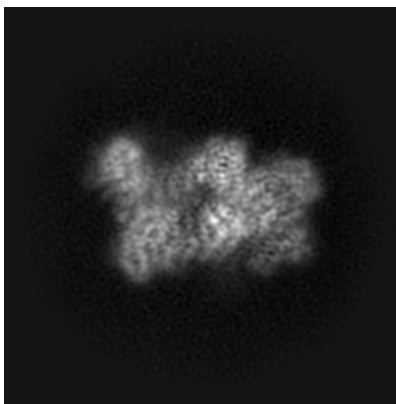
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

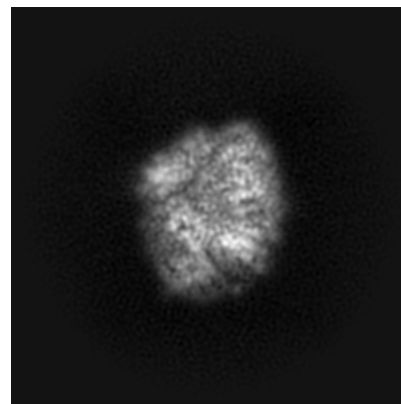
6.1.1 Primary map



X

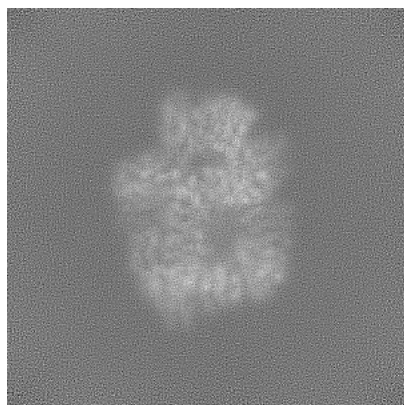


Y

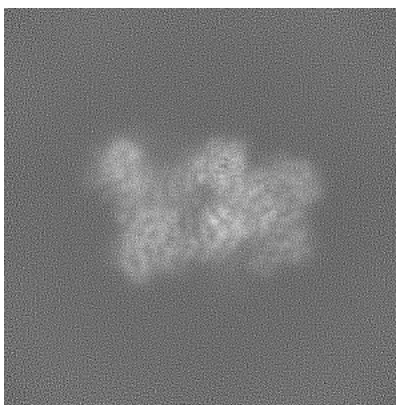


Z

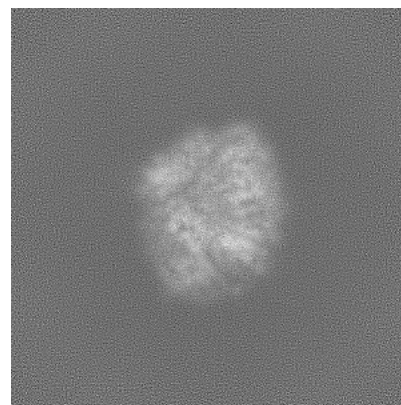
6.1.2 Raw map



X



Y

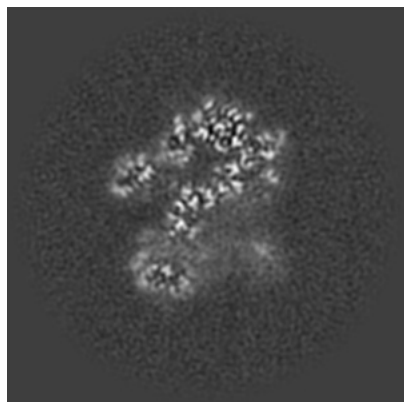


Z

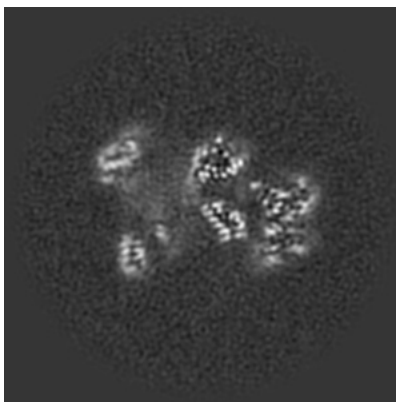
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

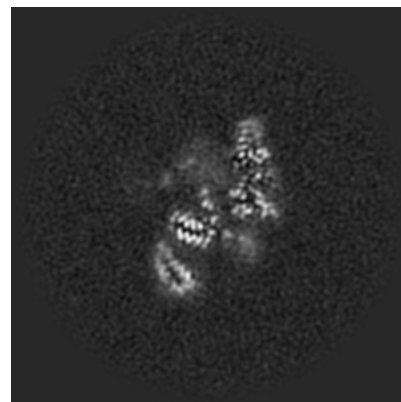
6.2.1 Primary map



X Index: 215

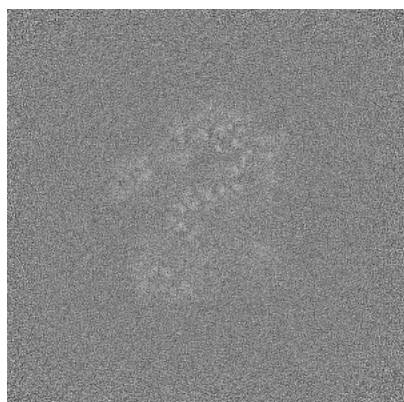


Y Index: 215

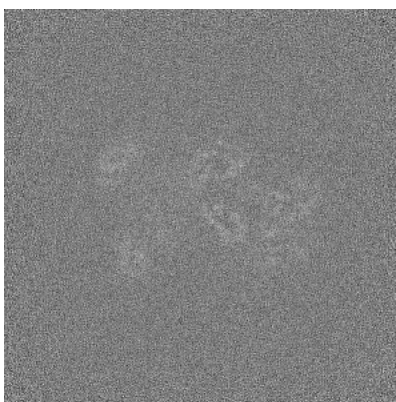


Z Index: 215

6.2.2 Raw map



X Index: 215



Y Index: 215

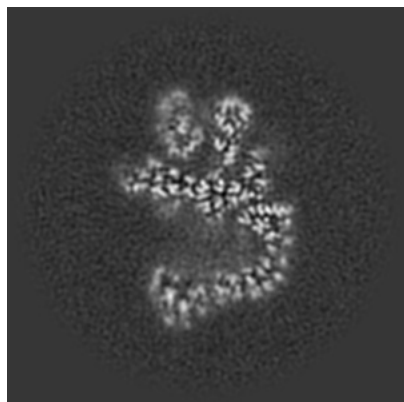


Z Index: 215

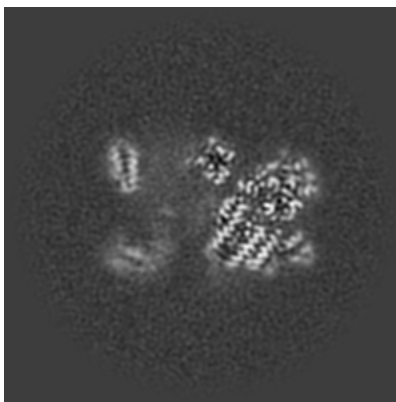
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

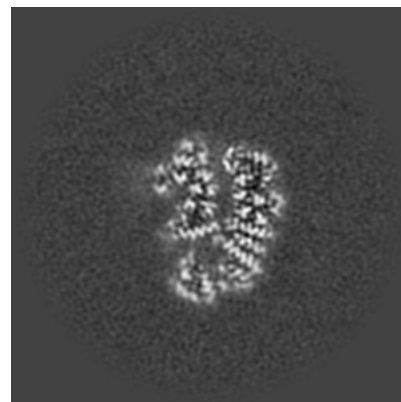
6.3.1 Primary map



X Index: 249

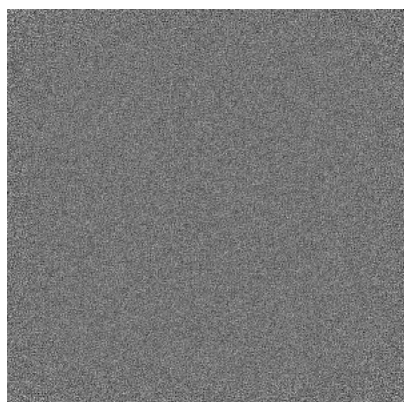


Y Index: 245

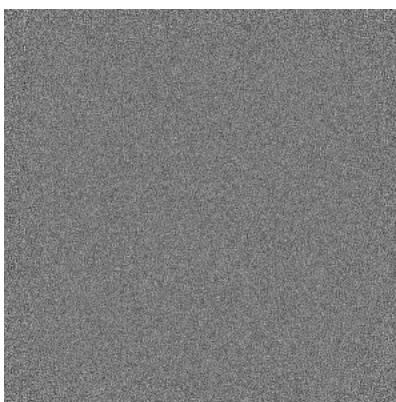


Z Index: 233

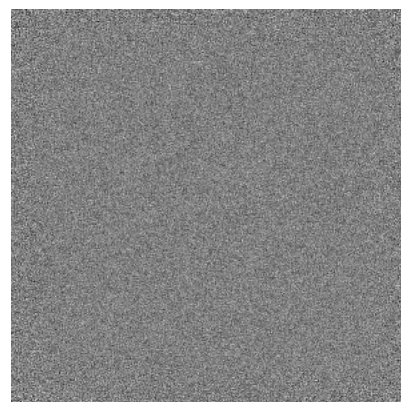
6.3.2 Raw map



X Index: 0



Y Index: 0

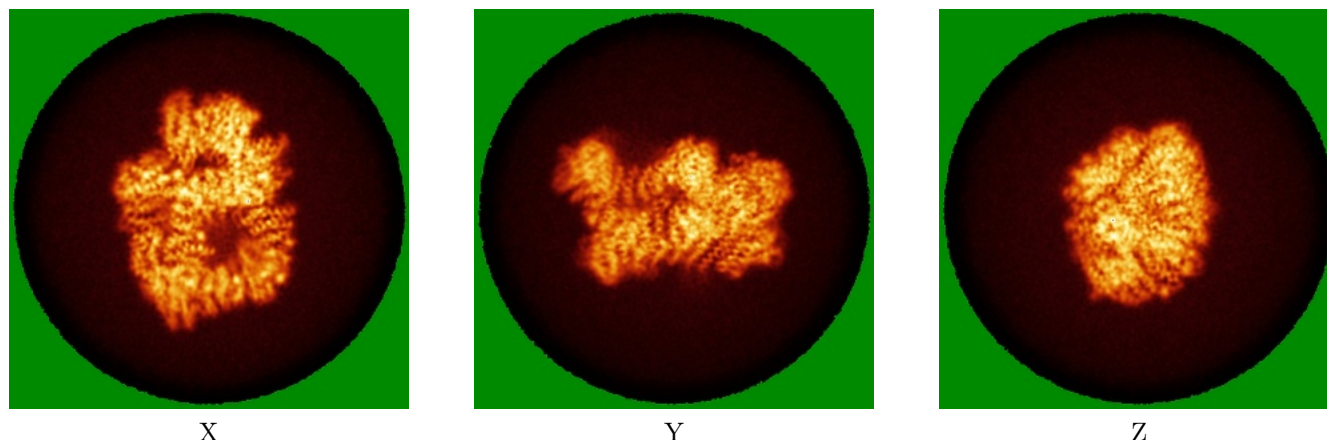


Z Index: 0

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

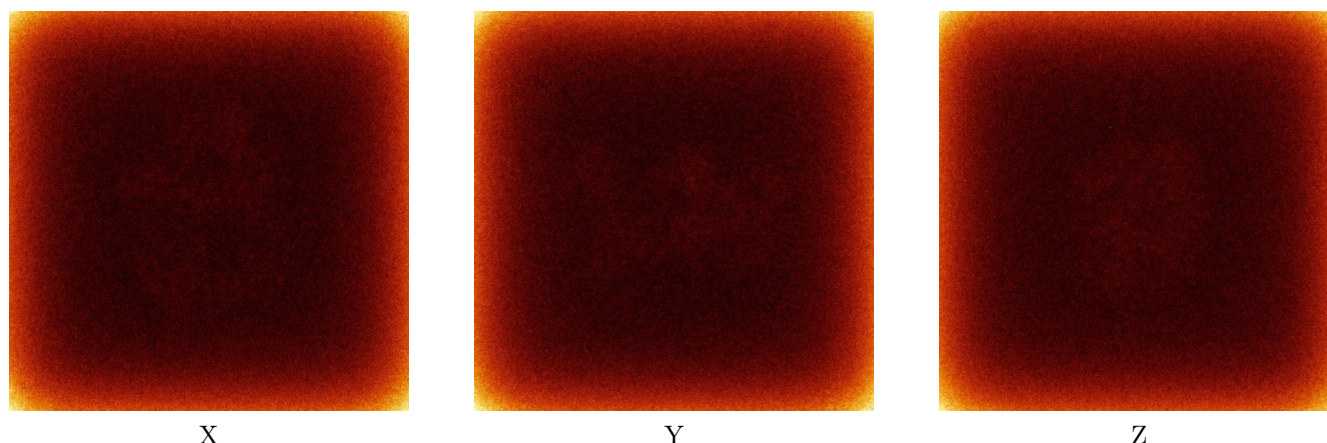


X

Y

Z

6.4.2 Raw map



X

Y

Z

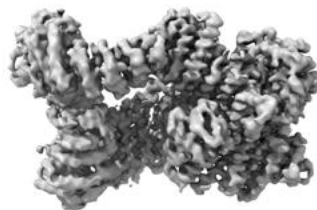
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

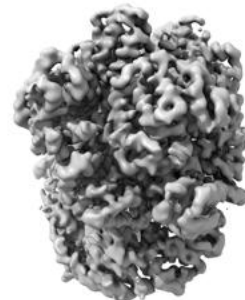
6.5.1 Primary map



X



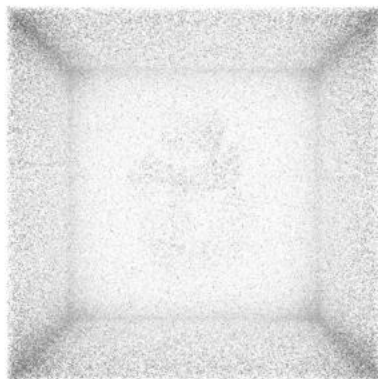
Y



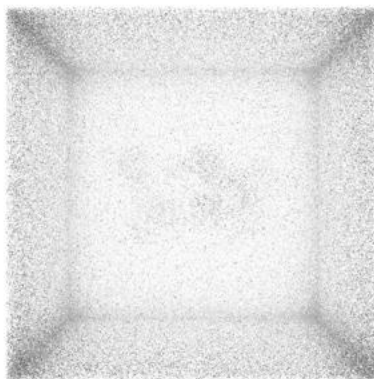
Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

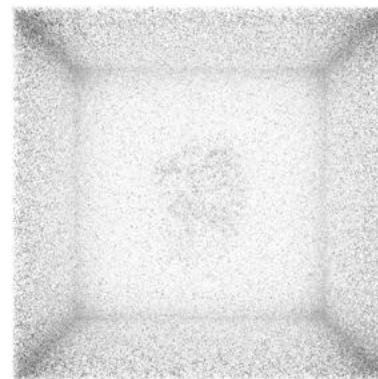
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

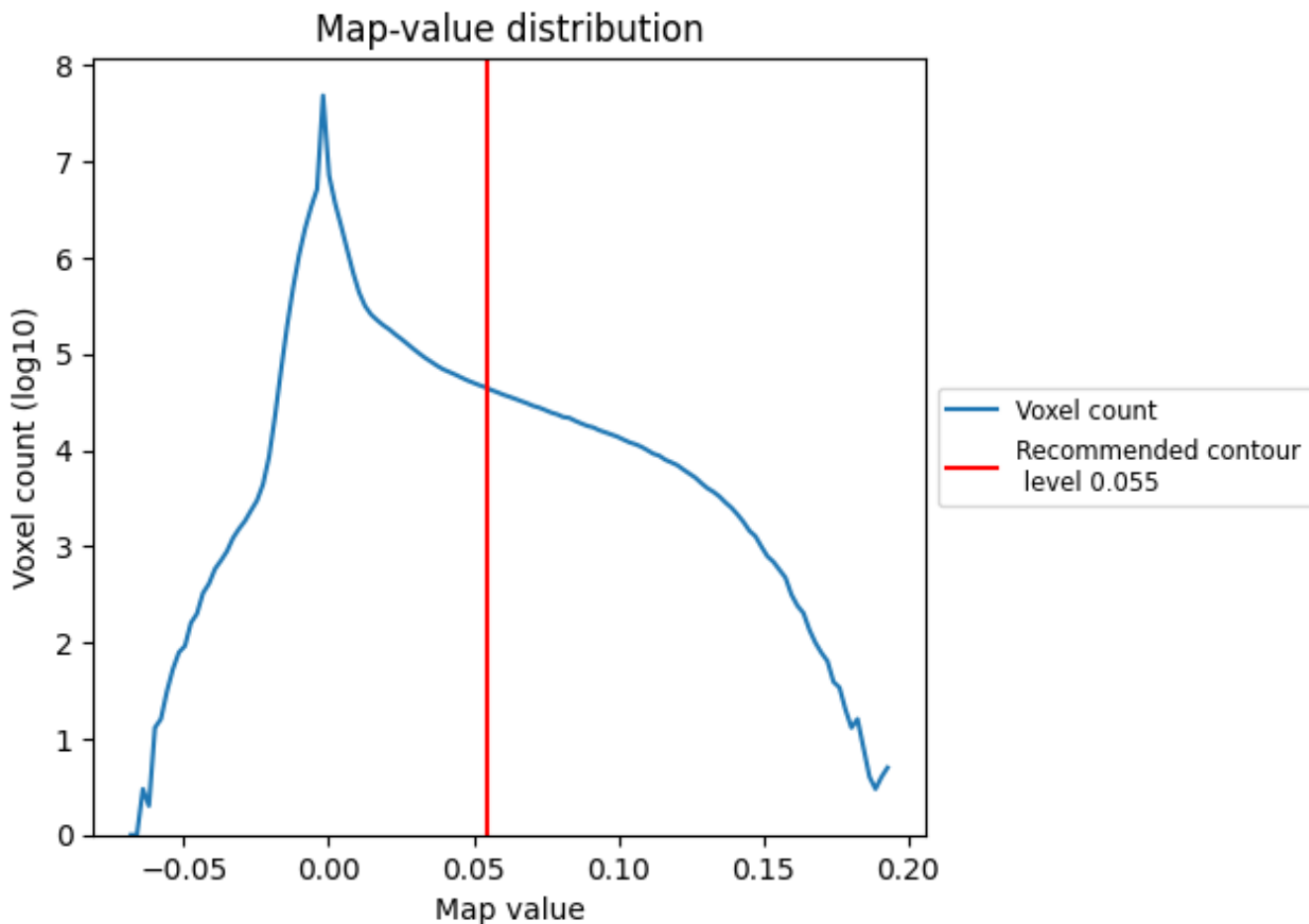
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

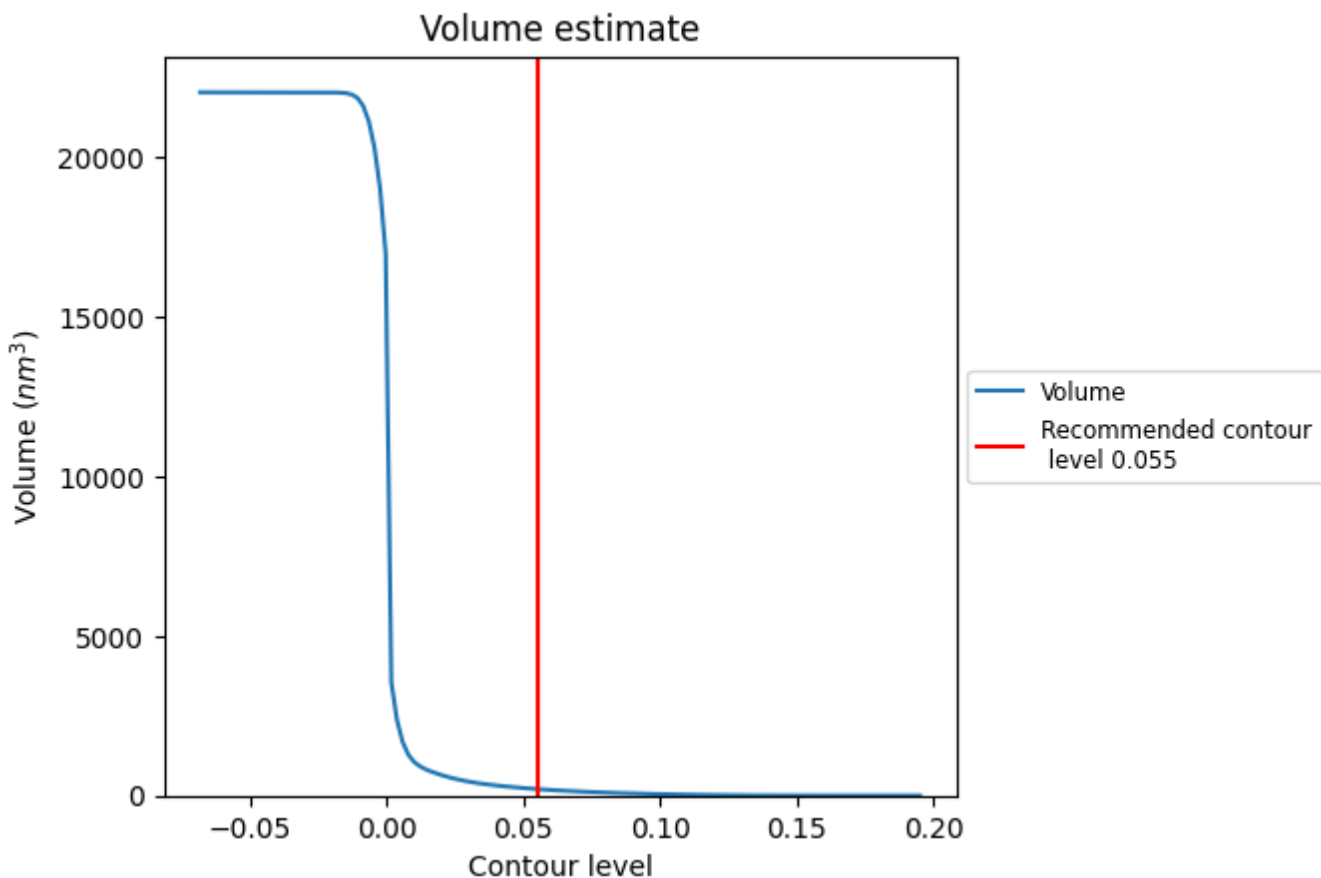
This section contains the results of statistical analysis of the map.

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.

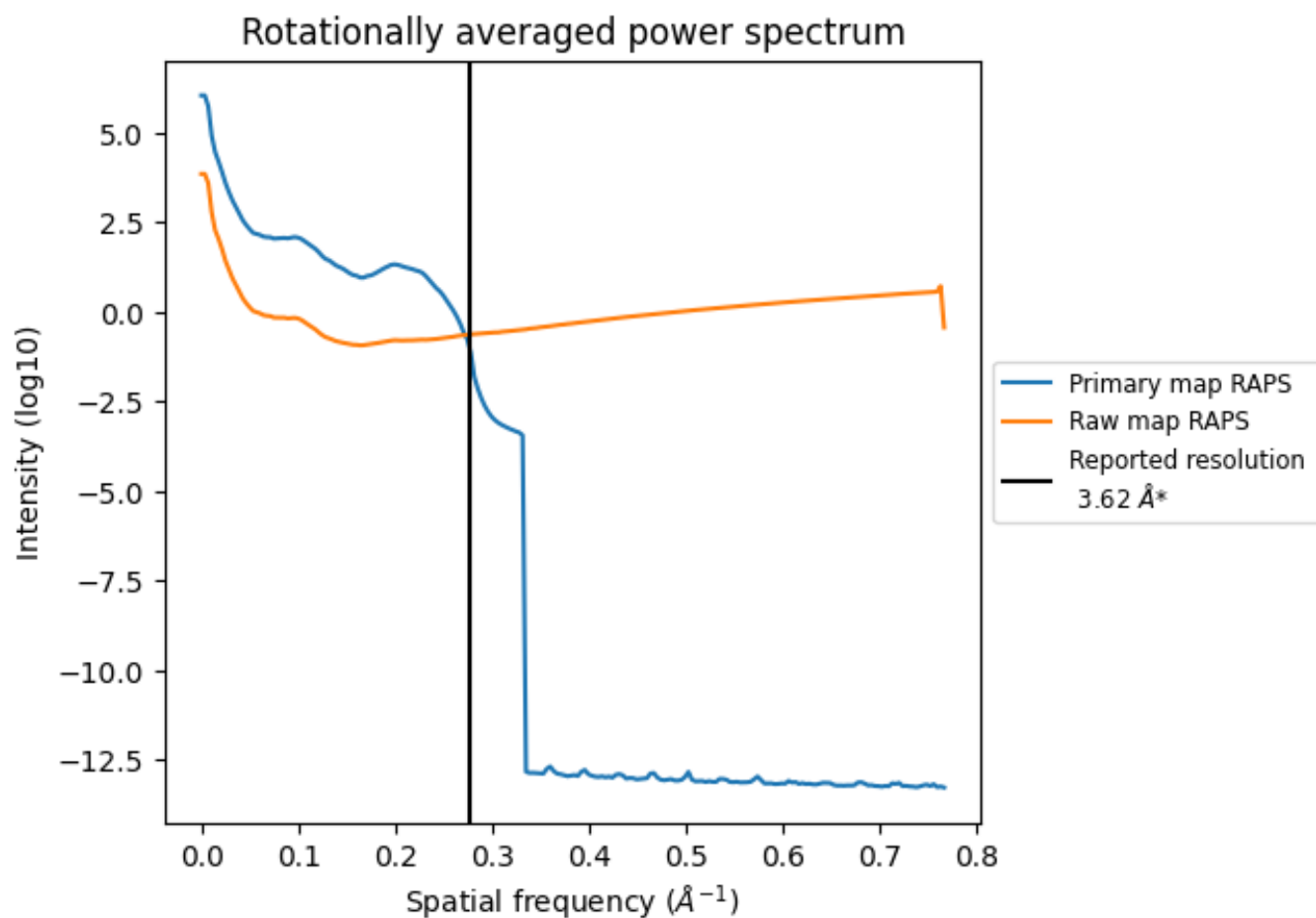
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

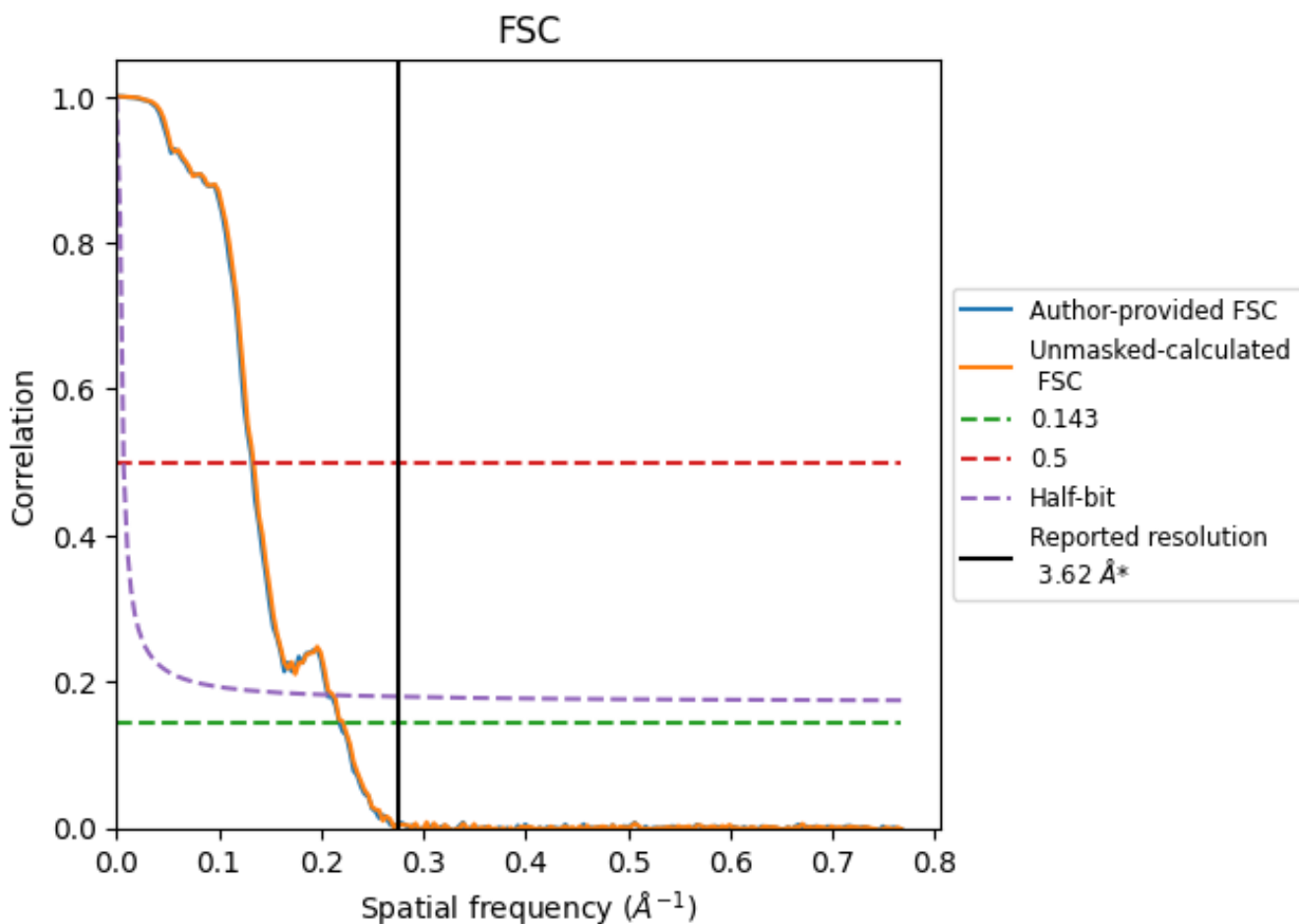


*Reported resolution corresponds to spatial frequency of 0.276 \AA^{-1}

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 0.276 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	4.58	7.55	4.84
Unmasked-calculated*	4.51	7.47	4.73

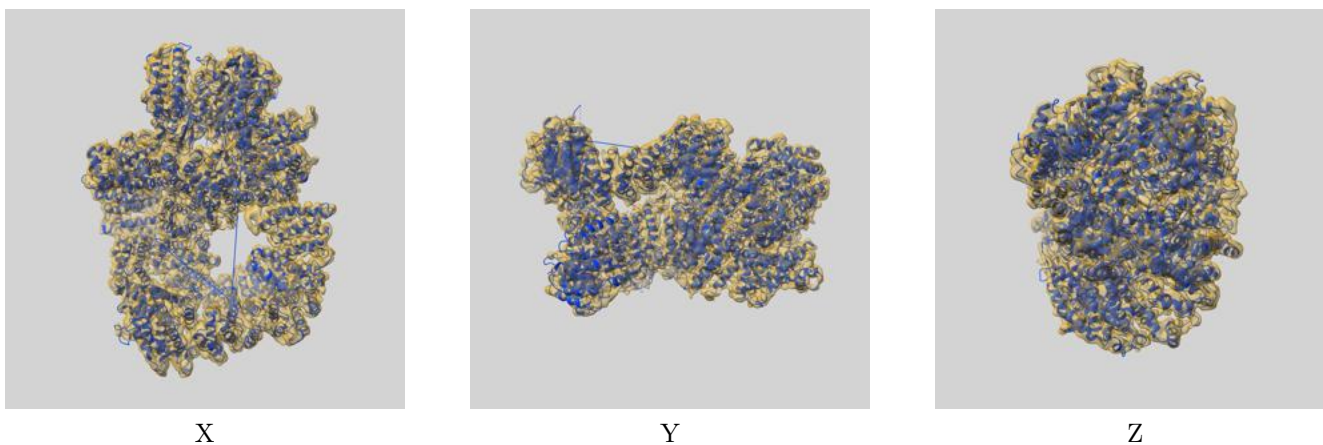
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.58 differs from the reported value 3.62 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.62 by more than 10 %

9 Map-model fit [i](#)

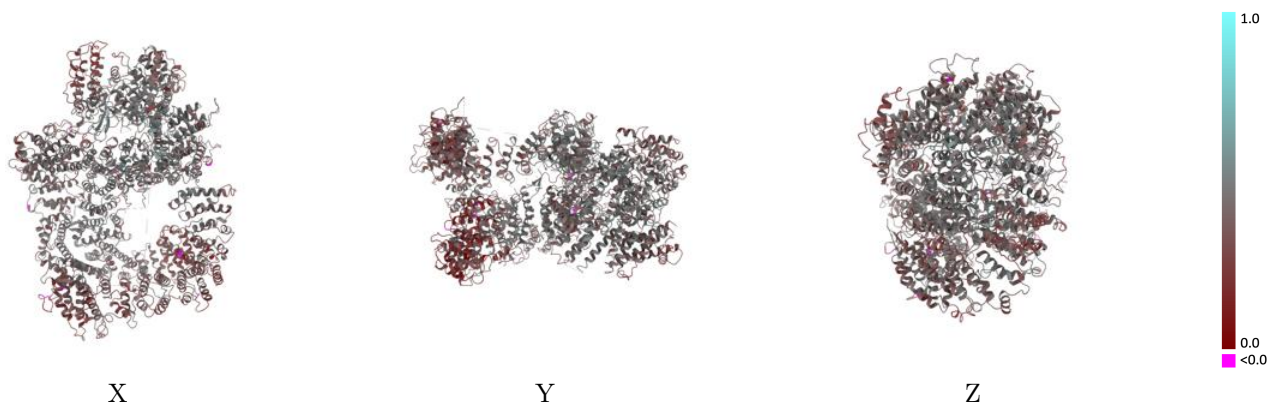
This section contains information regarding the fit between EMDB map EMD-11213 and PDB model 6ZH4. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



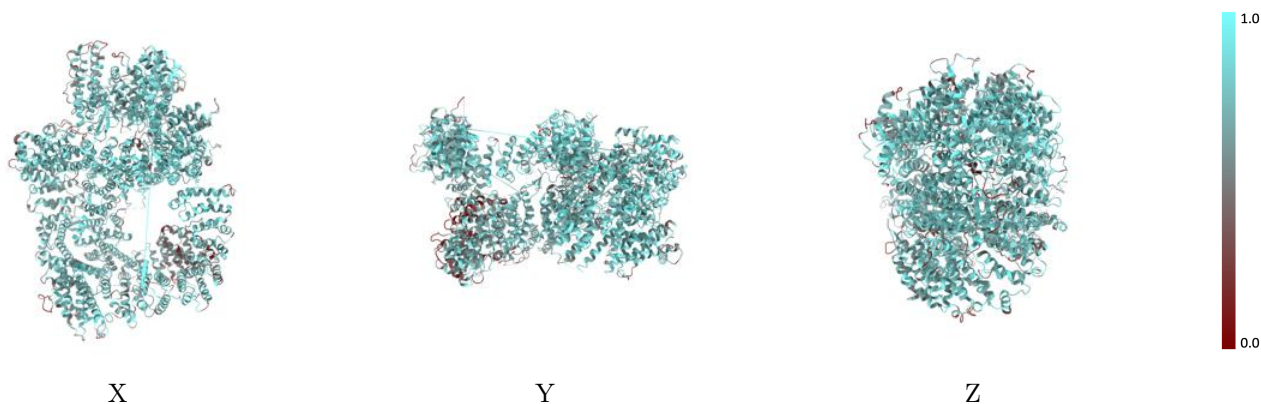
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



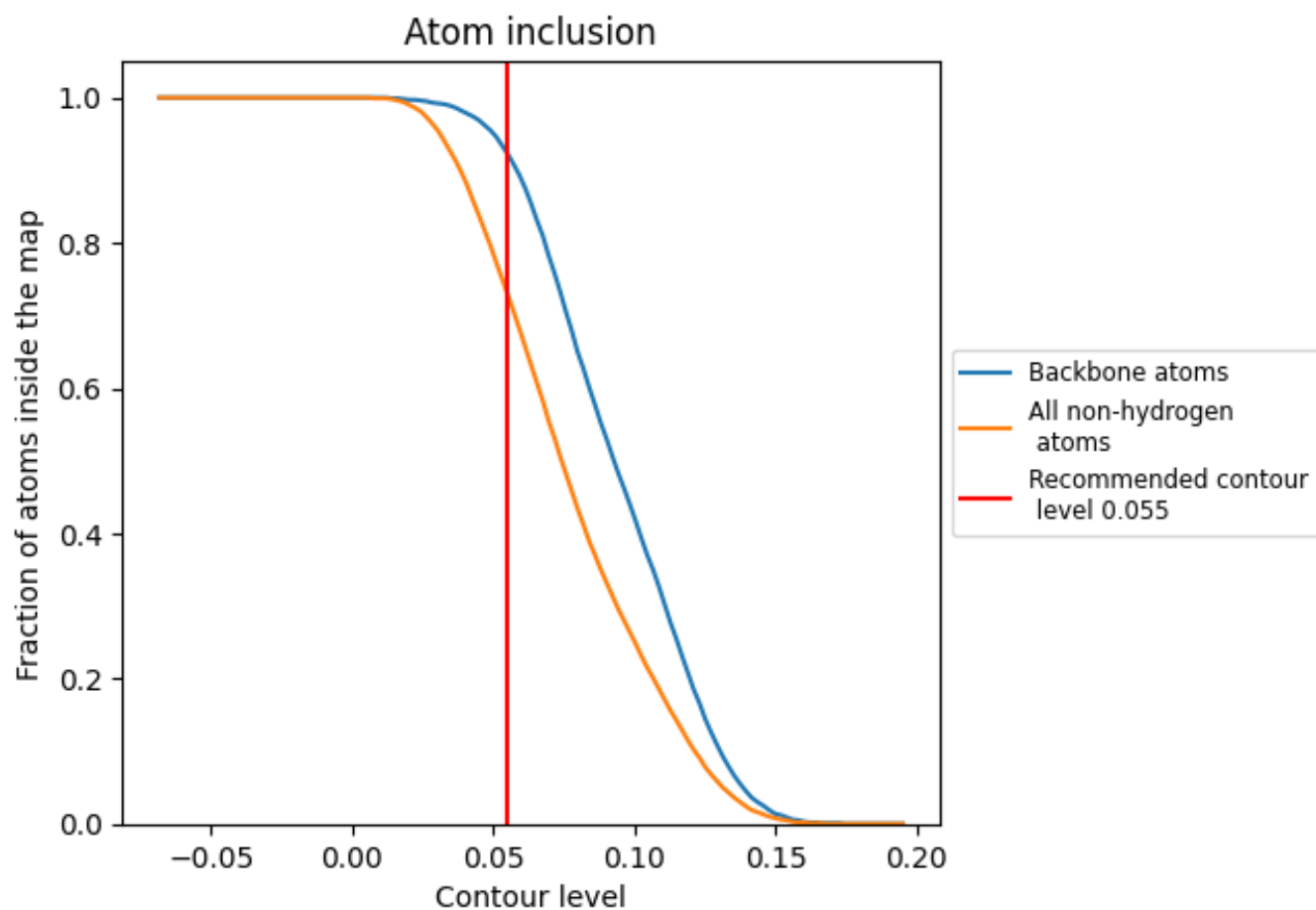
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).





9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 0.3980
A	 0.7300	 0.3980

