



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 09:00 AM EST

PDB ID : 7TYR
EMDB ID : EMD-26192
Title : Cryo-EM structure of the basal state of the Artemis:DNA-PKcs complex (see COMPND 13/14)
Authors : Watanabe, G.; Lieber, M.R.; Williams, D.R.
Deposited on : 2022-02-14
Resolution : 3.33 Å (reported)
Based on initial model : 5LUQ

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

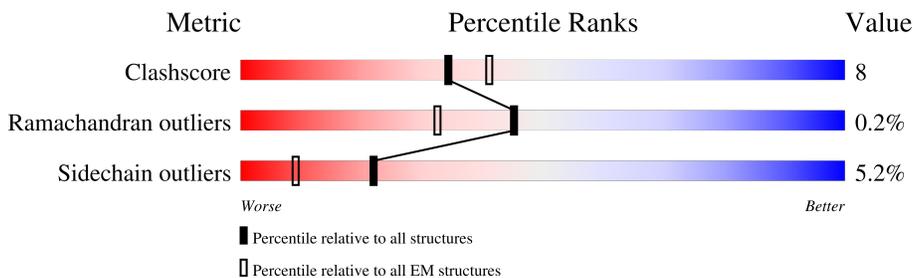
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4128	
2	C	707	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 31610 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3905	31173	19935	5272	5764	202	1	0

- Molecule 2 is a protein called Protein artemis.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	52	437	279	76	82	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	693	GLU	-	expression tag	UNP Q96SD1
C	694	ASN	-	expression tag	UNP Q96SD1
C	695	LEU	-	expression tag	UNP Q96SD1
C	696	TYR	-	expression tag	UNP Q96SD1
C	697	PHE	-	expression tag	UNP Q96SD1
C	698	GLN	-	expression tag	UNP Q96SD1
C	699	GLY	-	expression tag	UNP Q96SD1
C	700	HIS	-	expression tag	UNP Q96SD1
C	701	HIS	-	expression tag	UNP Q96SD1
C	702	HIS	-	expression tag	UNP Q96SD1
C	703	HIS	-	expression tag	UNP Q96SD1
C	704	HIS	-	expression tag	UNP Q96SD1
C	705	HIS	-	expression tag	UNP Q96SD1
C	706	HIS	-	expression tag	UNP Q96SD1
C	707	HIS	-	expression tag	UNP Q96SD1

LEU	M1071	V1217	M1401	L1531	L1710	K1852	L1984	P2059	M2126	M2305	V2423	L2581	THR
THR	K1074	L1220	K1407	L1532	R1711	F1855	L1987	R2060	K2132	K2313	M2424	F2588	THR
GLN	A1081	L1221	Y1411	L1538	L1714	T1856	Y1988	P2061	R2143	E2314	R2425	R2426	THR
ALA	F1082	G1234	Y1411	A1541	Q1716	K1857	M1989	A2062	R2143	A2318	R2427	D2428	ASP
ASP	M1083	L1236	T1424	S1542	L1717	L1858	F1990	Z2063	L2149	V2322	D2429	D2430	GLY
GLY	M1084	L1236	Q1426	L1543	P1723	M1859	F1991	G2064	V2150	G2324	E2431	E2431	ARG
ARG	M1085	P1239	Q1426	G1544	Q1725	E1860	VAL	R2065	E2154	L2323	R2431	D2438	SER
SER	M1086	T1240	Q1442	S1545	M1724	K1869	GLU	R2066	E2155	L2324	E2438	E2450	SER
SER	M1087	L1241	Q1444	S1546	Q1725	K1870	VAL	R2067	V2166	L2325	E2438	E2450	ASP
PHE	M1090	L1241	R1443	Q1547	M1738	M1871	VAL	R2068	V2166	L2326	E2438	E2450	ASP
THR	R1097	Y1243	R1445	G1548	M1738	M1871	VAL	R2069	F2157	L2327	E2438	E2450	THR
GLY	Q1098	L1254	L1448	L1562	A1749	I1876	PRO	E2070	R2158	L2328	E2438	E2450	GLY
SER	F1099	L1259	V1452	I1567	L1750	I1879	MET	GLN	P2159	L2329	E2438	E2450	SER
THR	E1102	L1264	H1459	E1570	S1753	M1880	ARG	ARG	A2161	L2330	E2438	E2450	SER
ASP	L1134	L1264	H1459	E1570	M1762	D1888	GLU	ASP	K2162	L2331	E2438	E2450	THR
PRO	I1138	Y1267	L1463	N1574	V1765	D1888	GLU	THR	H2163	L2332	E2438	E2450	THR
LEU	Y1268	T1269	L1466	N1589	R1768	E1893	LYS	THR	L2165	L2333	E2438	E2450	ASP
LEU	P1154	F1296	M1466	T1590	R1768	F1900	LYS	ASP	H2165	L2334	E2438	E2450	ASP
LEU	P1159	F1296	M1466	S1594	R1768	H1901	LYS	ASP	L2166	L2335	E2438	E2450	ASP
LEU	L1163	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2336	E2438	E2450	ASP
LEU	L1165	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2337	E2438	E2450	ASP
LEU	L1169	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2338	E2438	E2450	ASP
LEU	L1172	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2339	E2438	E2450	ASP
LEU	R1178	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2340	E2438	E2450	ASP
LEU	K1186	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2341	E2438	E2450	ASP
LEU	S1187	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2342	E2438	E2450	ASP
LEU	I1188	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2343	E2438	E2450	ASP
LEU	E1189	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2344	E2438	E2450	ASP
LEU	L1190	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2345	E2438	E2450	ASP
LEU	R1202	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2346	E2438	E2450	ASP
LEU	L1206	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2347	E2438	E2450	ASP
LEU	W1207	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2348	E2438	E2450	ASP
LEU	K1209	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2349	E2438	E2450	ASP
LEU	D1210	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2350	E2438	E2450	ASP
LEU	Y1211	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2351	E2438	E2450	ASP
LEU	L1212	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2352	E2438	E2450	ASP
LEU	K1213	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2353	E2438	E2450	ASP
LEU	E1215	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2354	E2438	E2450	ASP
LEU	G1216	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2355	E2438	E2450	ASP
LEU	D1397	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2356	E2438	E2450	ASP
LEU	L1301	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2357	E2438	E2450	ASP
LEU	C1312	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2358	E2438	E2450	ASP
LEU	F1313	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2359	E2438	E2450	ASP
LEU	G1314	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2360	E2438	E2450	ASP
LEU	T1315	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2361	E2438	E2450	ASP
LEU	G1316	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2362	E2438	E2450	ASP
LEU	A1317	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2363	E2438	E2450	ASP
LEU	G1499	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2364	E2438	E2450	ASP
LEU	L1500	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2365	E2438	E2450	ASP
LEU	P1501	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2366	E2438	E2450	ASP
LEU	S1502	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2367	E2438	E2450	ASP
LEU	L1503	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2368	E2438	E2450	ASP
LEU	K1508	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2369	E2438	E2450	ASP
LEU	L1514	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2370	E2438	E2450	ASP
LEU	L1515	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2371	E2438	E2450	ASP
LEU	E1516	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2372	E2438	E2450	ASP
LEU	L1517	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2373	E2438	E2450	ASP
LEU	A1518	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2374	E2438	E2450	ASP
LEU	F1519	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2375	E2438	E2450	ASP
LEU	A1520	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2376	E2438	E2450	ASP
LEU	L1524	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2377	E2438	E2450	ASP
LEU	C1525	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2378	E2438	E2450	ASP
LEU	F1526	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2379	E2438	E2450	ASP
LEU	L1528	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2380	E2438	E2450	ASP
LEU	V1529	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2381	E2438	E2450	ASP
LEU	S1530	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2382	E2438	E2450	ASP
LEU	L1639	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2383	E2438	E2450	ASP
LEU	M1643	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2384	E2438	E2450	ASP
LEU	A1644	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2385	E2438	E2450	ASP
LEU	V1645	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2386	E2438	E2450	ASP
LEU	H1685	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2387	E2438	E2450	ASP
LEU	Y1675	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2388	E2438	E2450	ASP
LEU	D1685	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2389	E2438	E2450	ASP
LEU	L1686	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2390	E2438	E2450	ASP
LEU	K1689	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2391	E2438	E2450	ASP
LEU	A1692	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2392	E2438	E2450	ASP
LEU	L1696	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2393	E2438	E2450	ASP
LEU	S1706	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2394	E2438	E2450	ASP
LEU	L1790	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2395	E2438	E2450	ASP
LEU	C1791	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2396	E2438	E2450	ASP
LEU	Q1794	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2397	E2438	E2450	ASP
LEU	V1795	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2398	E2438	E2450	ASP
LEU	G1796	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2399	E2438	E2450	ASP
LEU	L1797	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2400	E2438	E2450	ASP
LEU	V1801	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2401	E2438	E2450	ASP
LEU	V1820	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2402	E2438	E2450	ASP
LEU	L1824	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2403	E2438	E2450	ASP
LEU	L1828	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2404	E2438	E2450	ASP
LEU	S1832	F1296	M1466	S1594	R1768	G1902	ALA	ASP	L2166	L2405	E2438	E2450	ASP
LEU	R1837	F1296	M1466	S1594									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103485	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 ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46296	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.449	Depositor
Minimum map value	-1.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	552.96, 552.96, 552.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.29	0/31831	0.51	0/43042
2	C	0.56	0/452	0.67	0/614
All	All	0.29	0/32283	0.51	0/43656

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	31173	0	31434	479	0
2	C	437	0	424	35	0
All	All	31610	0	31858	501	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 501 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:C:381:VAL:HG13	2:C:382:HIS:ND1	1.35	1.35
2:C:381:VAL:CG1	2:C:382:HIS:ND1	2.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:365:THR:HG23	2:C:367:PRO:HD2	1.38	1.03
1:A:2911:ARG:CZ	1:A:2913:LYS:HE3	1.93	0.98
2:C:369:TYR:HB2	2:C:371:PRO:HD3	1.51	0.92

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	3896/4128 (94%)	3699 (95%)	191 (5%)	6 (0%)	44 72
2	C	50/707 (7%)	38 (76%)	11 (22%)	1 (2%)	6 29
All	All	3946/4835 (82%)	3737 (95%)	202 (5%)	7 (0%)	45 72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	SER
1	A	2161	ALA
1	A	2162	LYS
1	A	3716	HIS
1	A	682	TYR

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	3474/3671 (95%)	3312 (95%)	162 (5%)	22	51
2	C	50/647 (8%)	29 (58%)	21 (42%)	0	0
All	All	3524/4318 (82%)	3341 (95%)	183 (5%)	22	48

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2482	ASP
1	A	3588	TRP
1	A	2503	LYS
1	A	2962	ARG
1	A	3782	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2481	HIS
1	A	2977	ASN
1	A	1238	GLN
1	A	1611	GLN
1	A	1859	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

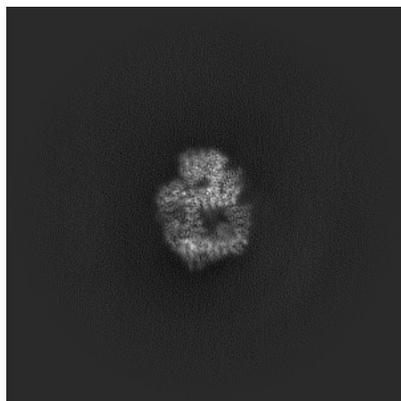
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26192. These allow visual inspection of the internal detail of the map and identification of artifacts.

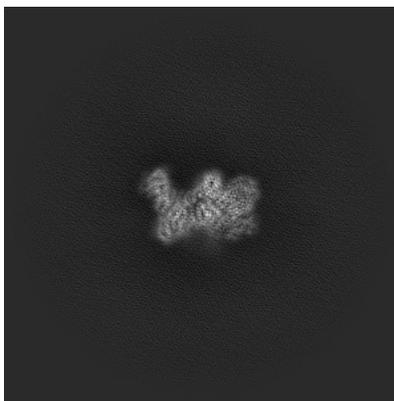
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

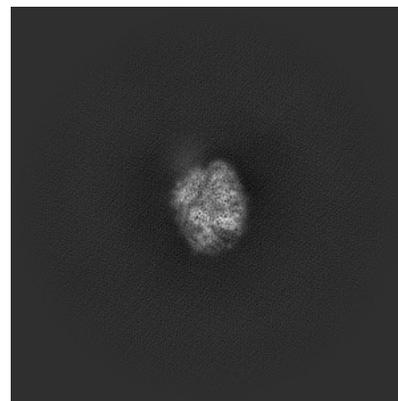
6.1.1 Primary map



X

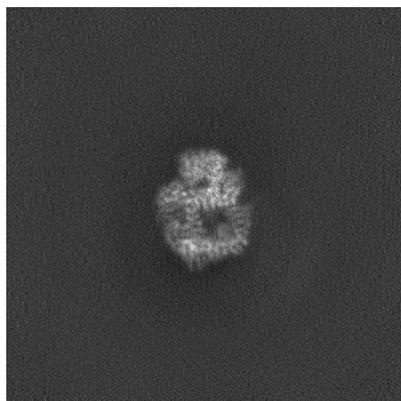


Y

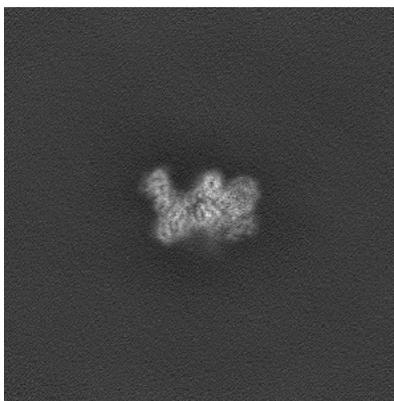


Z

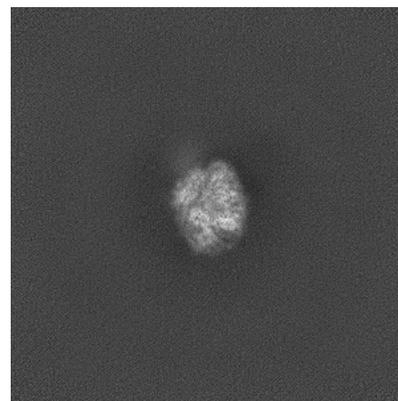
6.1.2 Raw map



X



Y

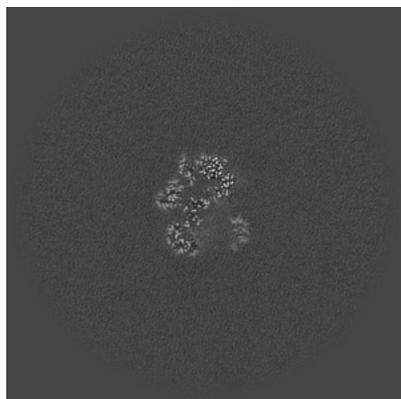


Z

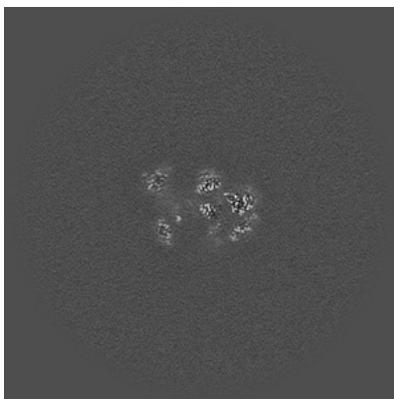
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256

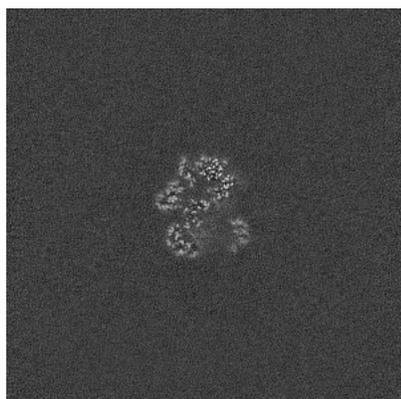


Y Index: 256

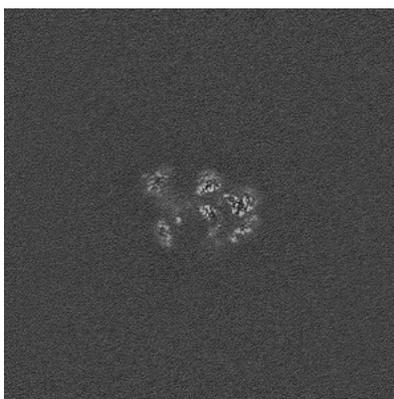


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

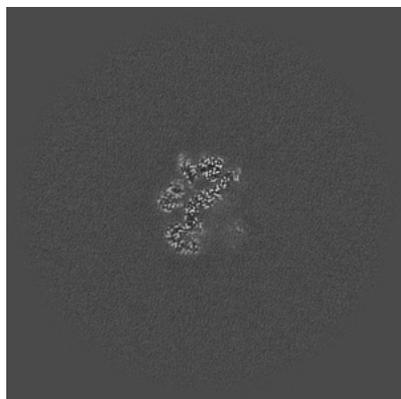


Z Index: 256

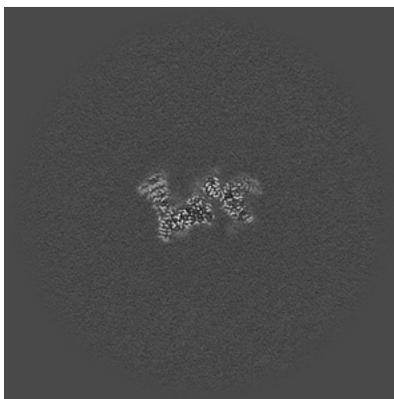
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

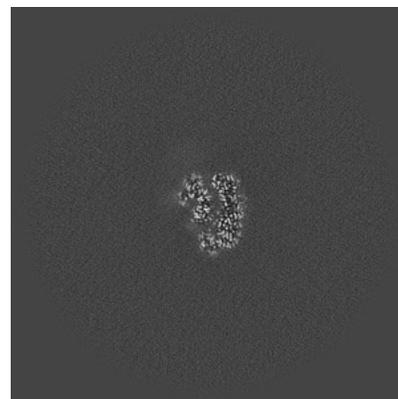
6.3.1 Primary map



X Index: 252

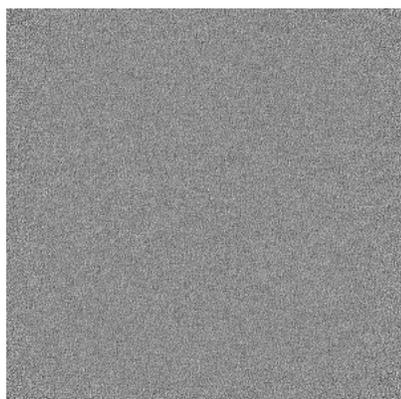


Y Index: 238

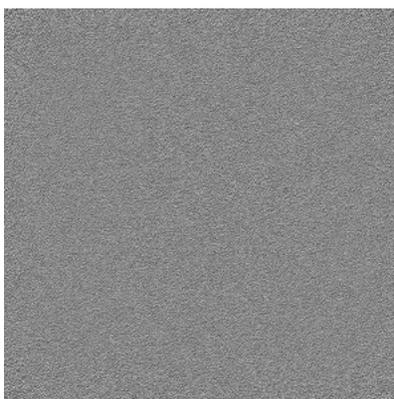


Z Index: 265

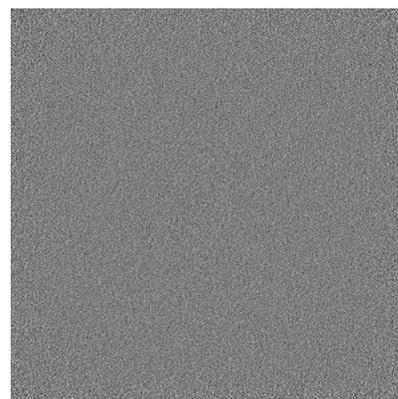
6.3.2 Raw map



X Index: 0



Y Index: 0

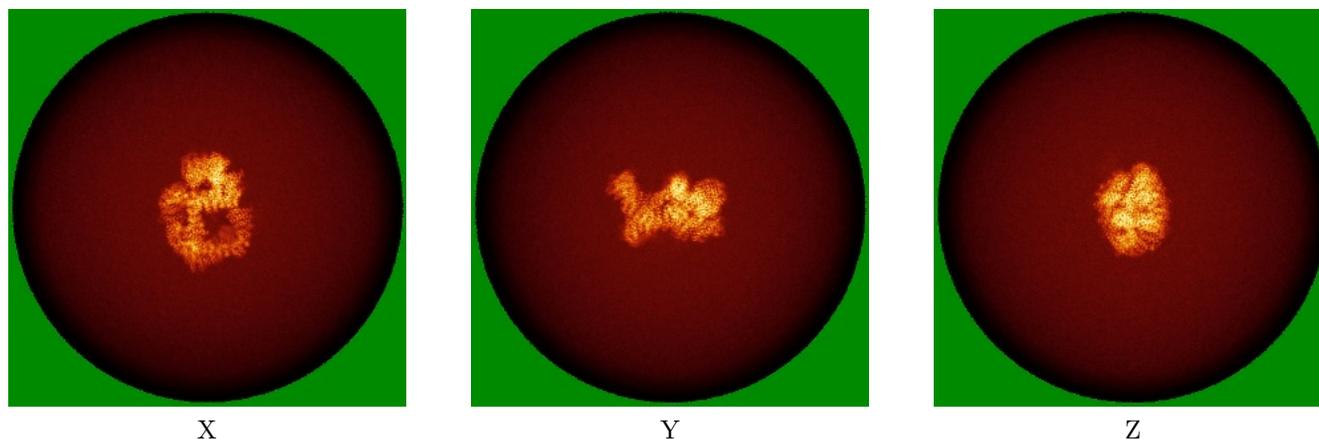


Z Index: 0

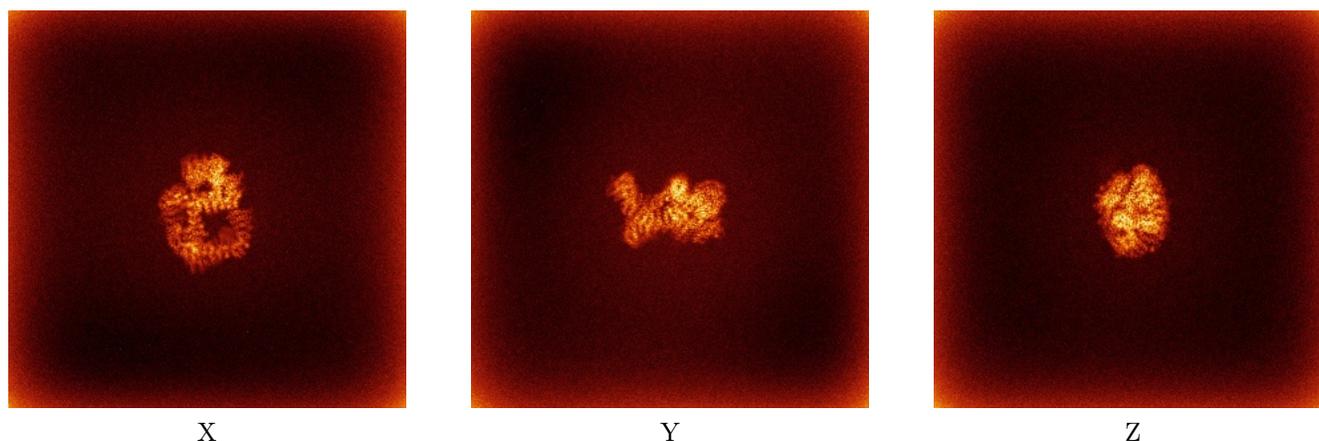
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

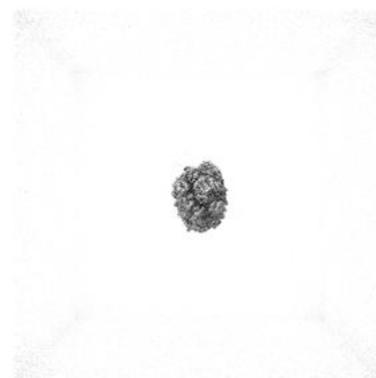
6.5.2 Raw map



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.

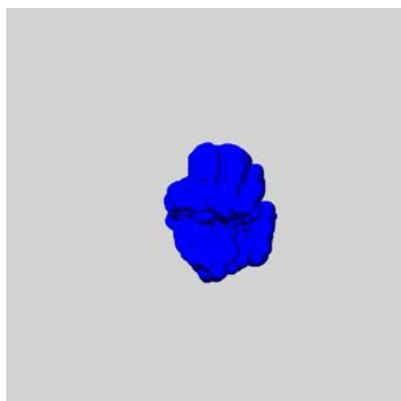
6.6 Mask visualisation [i](#)

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

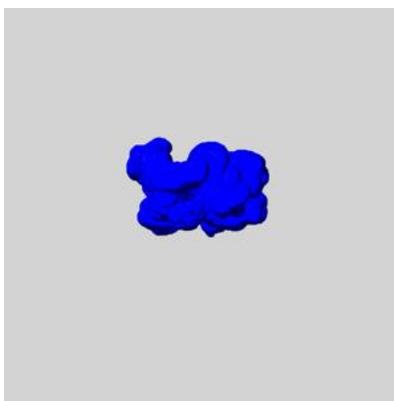
A mask typically either:

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

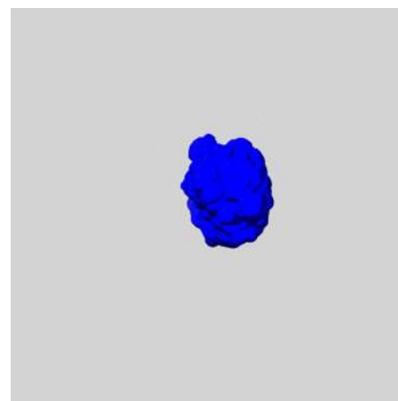
6.6.1 emd_26192_msk_1.map [i](#)



X



Y

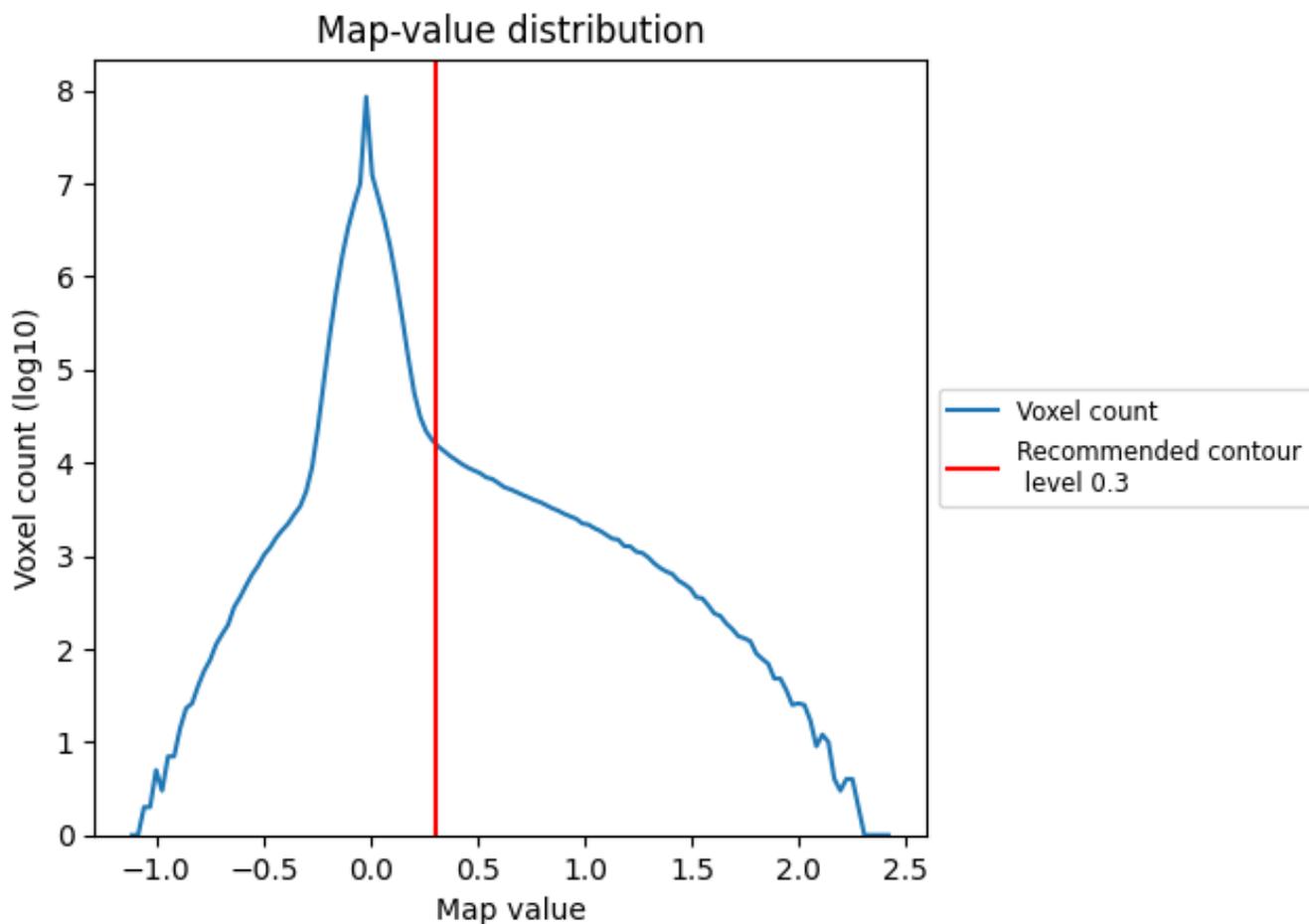


Z

7 Map analysis [i](#)

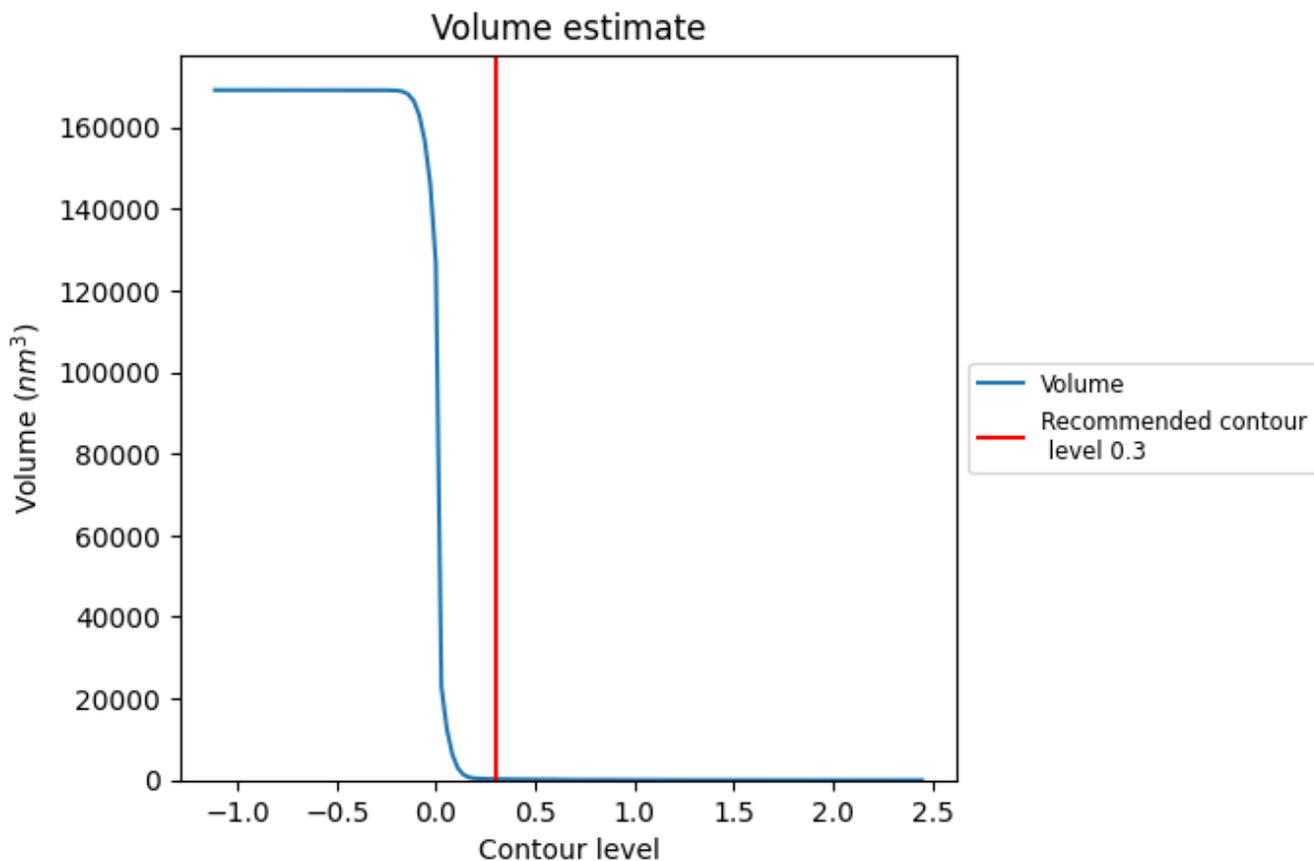
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

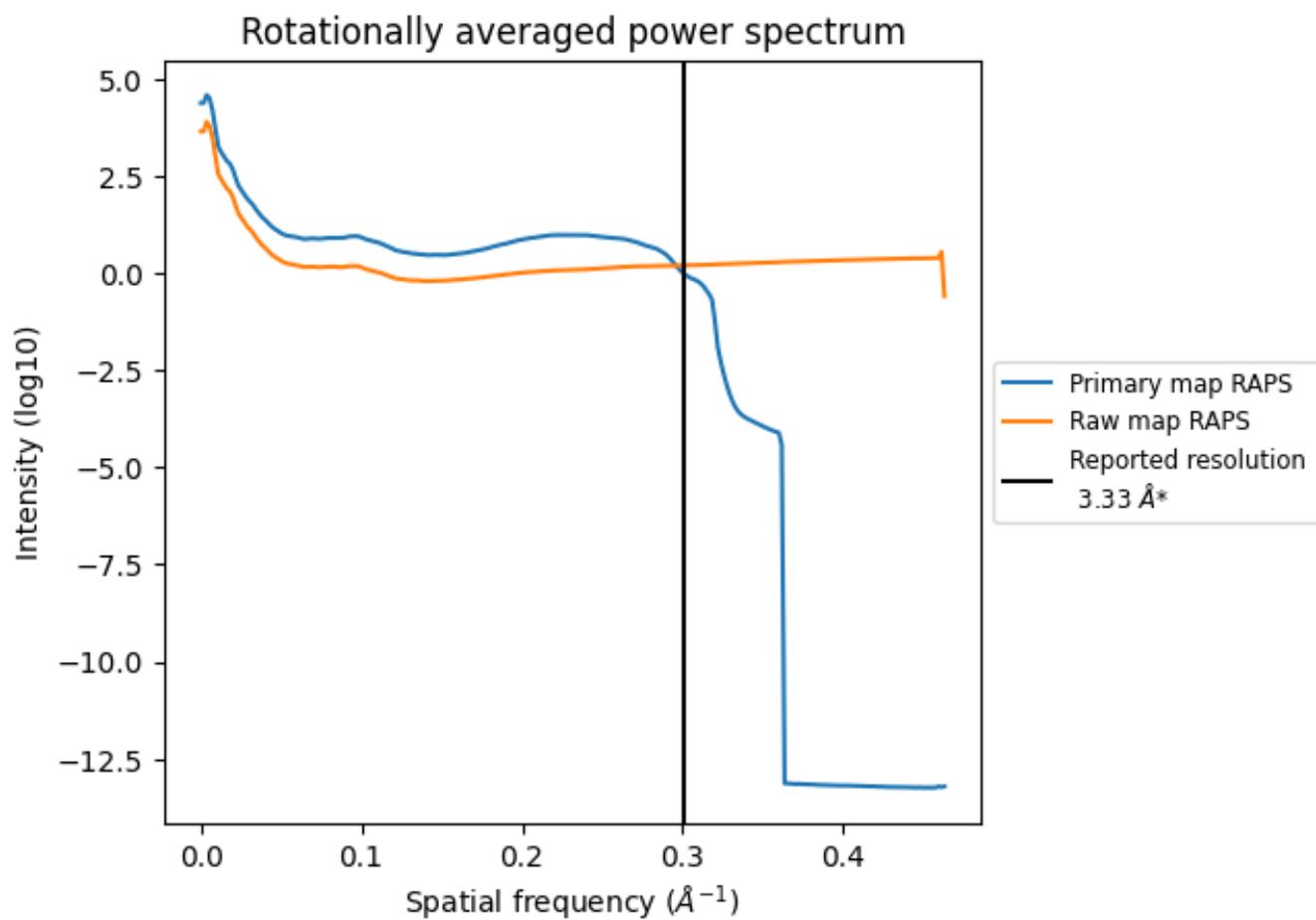
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 240 nm³; this corresponds to an approximate mass of 217 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](#)

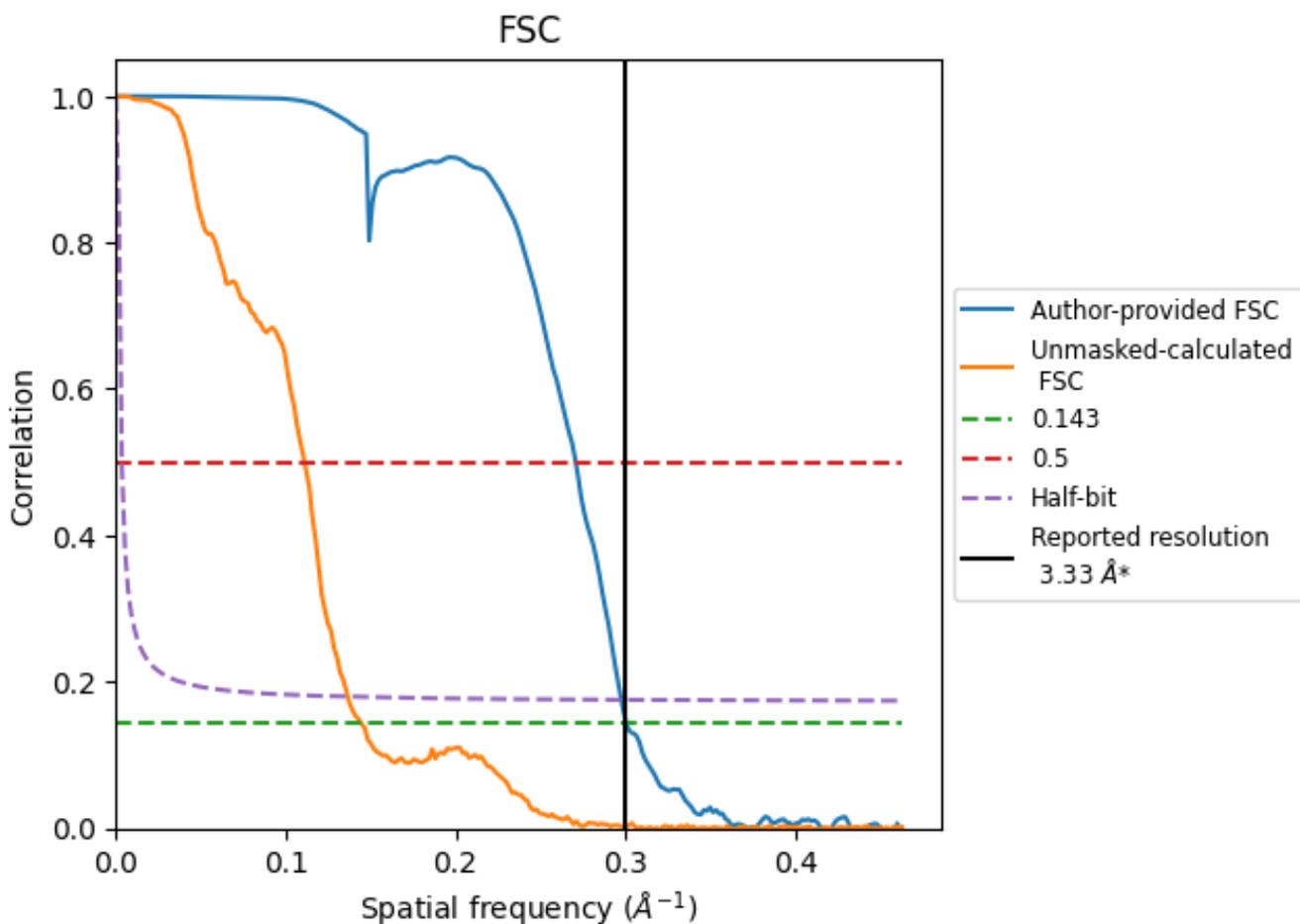


*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

8.2 Resolution estimates [i](#)

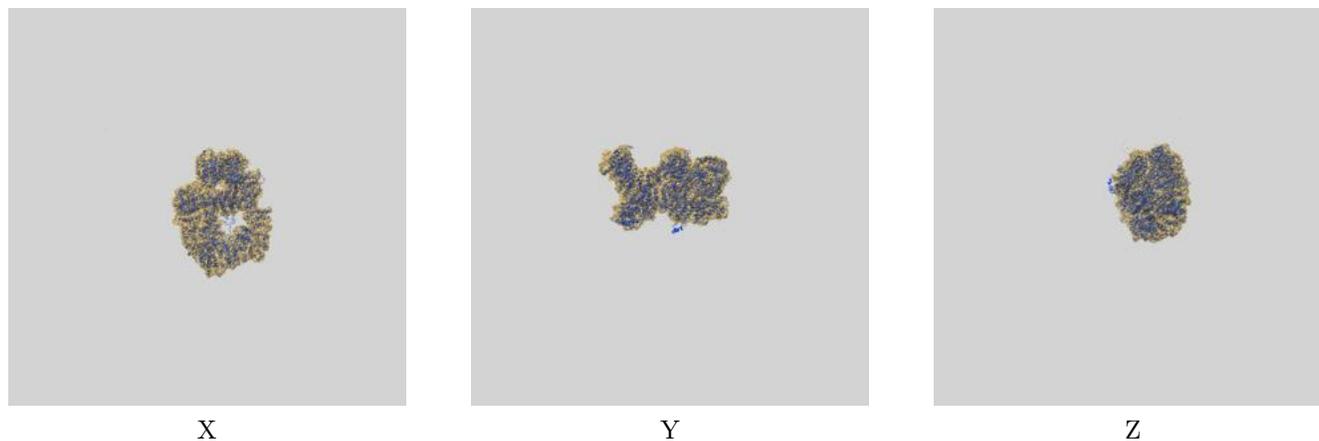
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.33	3.69	3.36
Unmasked-calculated*	6.93	9.00	7.32

*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 6.93 differs from the reported value 3.33 by more than 10 %

9 Map-model fit [i](#)

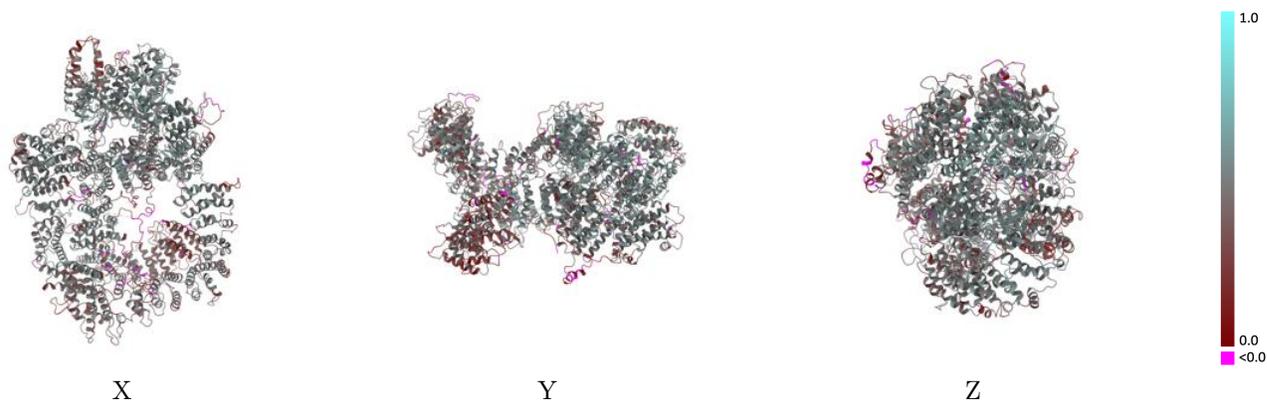
This section contains information regarding the fit between EMDB map EMD-26192 and PDB model 7TYR. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



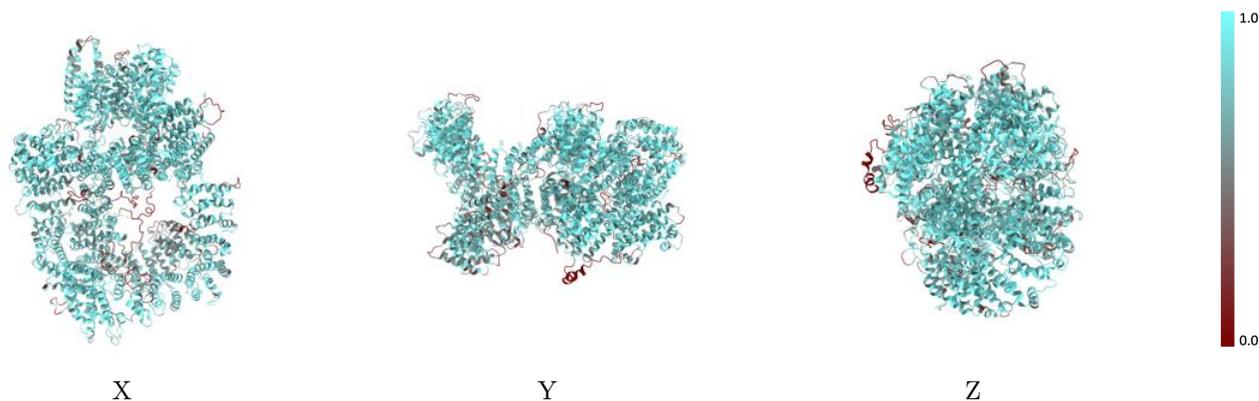
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



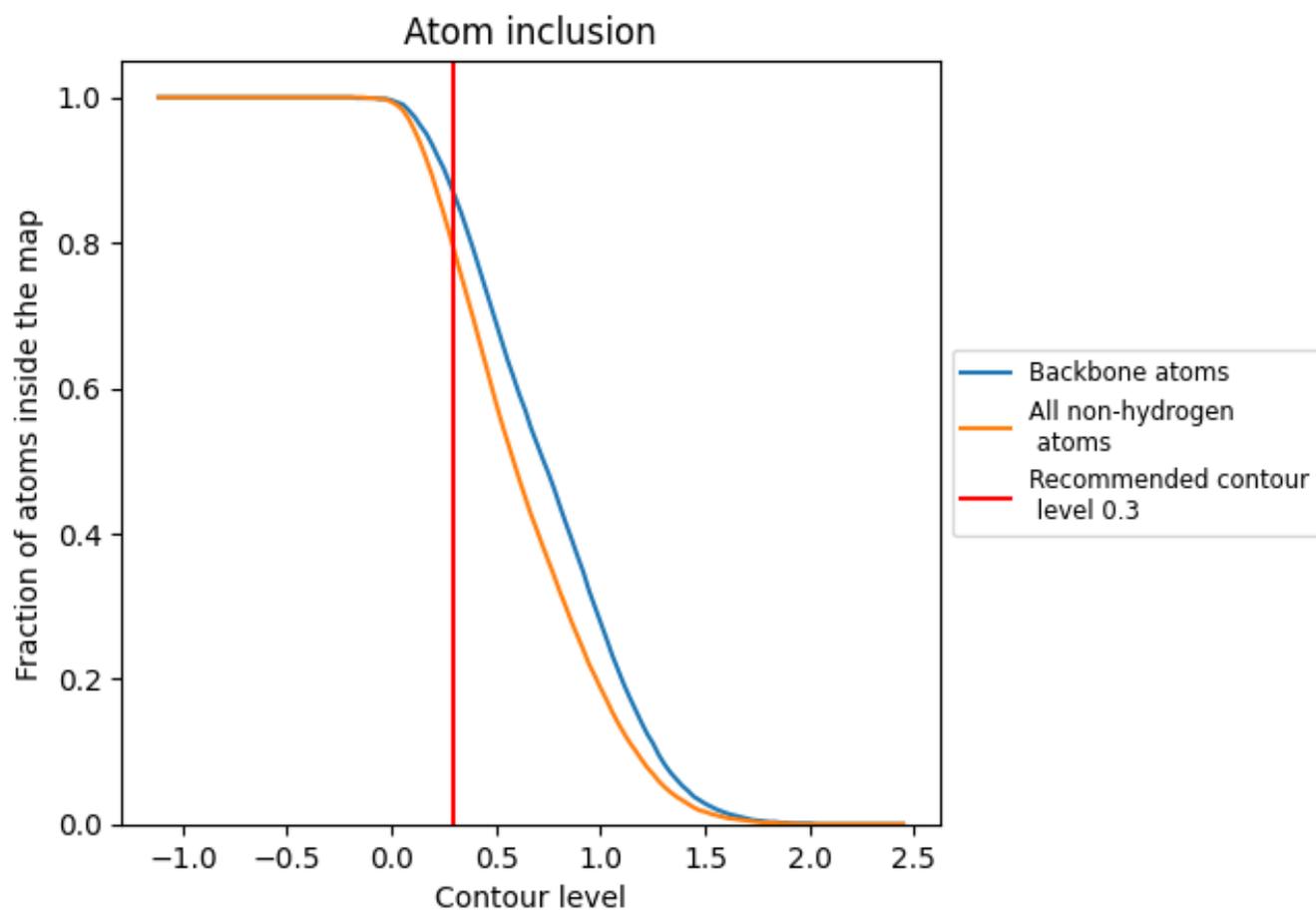
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7890	 0.4330
A	 0.7960	 0.4360
C	 0.3220	 0.2170

