



wwPDB EM Validation Summary Report ⓘ

May 6, 2025 – 11:10 AM EDT

PDB ID : 7UVK / pdb_00007uvk
EMDB ID : EMD-26812
Title : G. haemolysans IgA1 protease
Authors : Eisenmesser, E.Z.; Zheng, H.
Deposited on : 2022-05-02
Resolution : 3.28 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

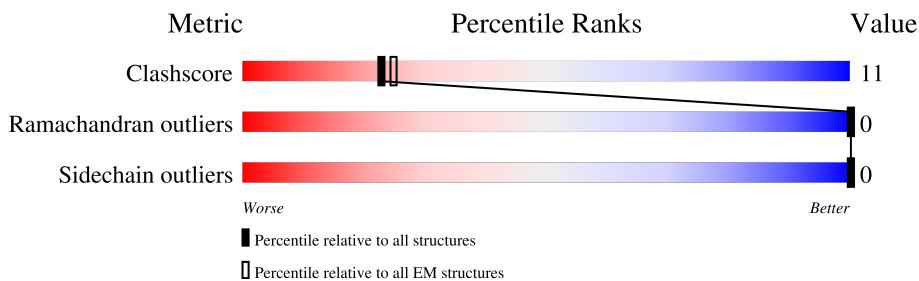
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.28 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	2201	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10350 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.

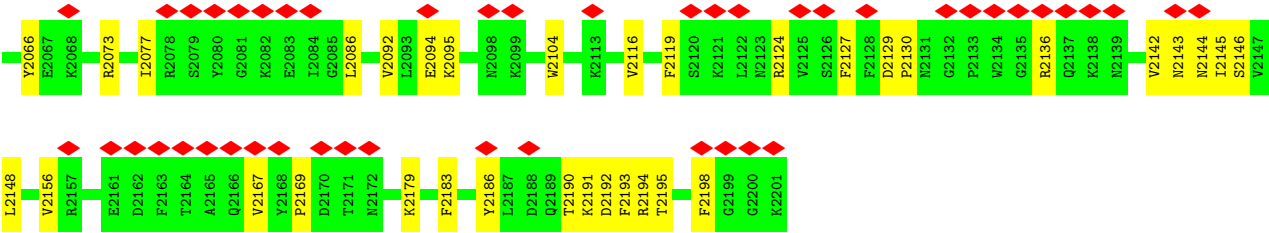
- Molecule 1 is a protein called IgA1 Protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1295	Total	C	N	O	S	0	0
			10350	6536	1750	2045	19		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP C5NYF3
A	2	ARG	-	expression tag	UNP C5NYF3
A	3	LYS	-	expression tag	UNP C5NYF3
A	4	TYR	-	expression tag	UNP C5NYF3
A	5	LEU	-	expression tag	UNP C5NYF3
A	6	GLU	-	expression tag	UNP C5NYF3
A	7	GLU	-	expression tag	UNP C5NYF3
A	8	LYS	-	expression tag	UNP C5NYF3
A	9	TYR	-	expression tag	UNP C5NYF3
A	10	ASN	-	expression tag	UNP C5NYF3
A	11	LYS	-	expression tag	UNP C5NYF3
A	12	PHE	-	expression tag	UNP C5NYF3
A	13	SER	-	expression tag	UNP C5NYF3
A	14	LEU	-	expression tag	UNP C5NYF3
A	15	ARG	-	expression tag	UNP C5NYF3
A	16	LYS	-	expression tag	UNP C5NYF3
A	17	LEU	-	expression tag	UNP C5NYF3
A	18	THR	-	expression tag	UNP C5NYF3
A	19	VAL	-	expression tag	UNP C5NYF3
A	20	GLY	-	expression tag	UNP C5NYF3
A	21	VAL	-	expression tag	UNP C5NYF3
A	22	CYS	-	expression tag	UNP C5NYF3
A	23	SER	-	expression tag	UNP C5NYF3

ALA	LEU	GLU	ARG	GLY	HIS	LYS	D907	E908	K909	K910	D911	D912	I913	K914	E915	E916	N1001	N1002	I1003	T1004	L1005	D920	L923	N927	N930	L933	L936	E937	N938	N939	K940	Y941	Y944	S945	S946	L947	S948	S949	V950	P951	T952	N953	P954	Y957	F958	N959	N965	D968	E977	S978	A979	R980																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
K981	D982	N983	Q984	D985	V990	A993	N994	D995	L996	I997	E1000	N1001	N1002	I1003	T1004	L1005	E1006	N1007	Y1008	T1009	F1013	K1014	T1015	V1016	N1017	N1018	E1019	N1020	G1021	V1022	Y1023	T1024	S1025	F1026	L1029	V1030	D1031	A1032	M1033	N1034	I1035	Y1038	L1043	G1044	M1047	D1048	A1049	R1050	E1051	V1052	E1053																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L1054	S1055	D1056	Q1057	Q1058	E1059	N1063	K1064	E1065	F1066	S1067	G1068	K1069	L1070	I1071	G1072	E1073	N1074	K1077	Y1078	Y1079	N1083	L1084	K1085	K1086	L1088	F1089	A1091	L1092	S1093	T1096	L1100	S1101	Y1107	S1108	E1111	A1114	A1117	K1118	T1135	A1136	R1139	S1140	T1141	I1145																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
V1148	I1153	T1159	I1162	D1167	T1168	A1169	T1170	T1171	Y1172	H1173	I1174	G1175	L1177	L1181	T1188	E1189	K1190	S1191	I1192	S1193	S1194	I1195	D1196	H1197	N1200	A1201	N1202	T1203	G1204	D1205	Q1206	V1207	V1208	V1211	V1214	V1215	D1216	A1219	Y1225	V1226	E1227	G1228	N1229	L1230	H1231	N1232																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
V1233	K1234	K1238	V1239	V1242	V1243	D1248	R1249	E1250	T1251	T1252	E1253	L1260	T1261	N1262	V1263	L1264	S1265	D1266	N1267	V1268	V1269	N1273	Y1278	D1279	F1280	N1281	A1285	T1286	N1287	S1290	N1291	K1292	V1296	V1297	V1300	Q1301	V1302	E1305	V1306	L1307	S1308	K1309	D1310	S1311	E1312	E1313	Q1314	R1315																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G1316	V1317	L1319	E1320	N1321	N1322	I1323	V1324	L1325	E1326	K1327	K1328	I1329	L1330	L1331	V1332	P1333	K1334	K1335	I1339	E1340	D1341	F1342	N1343	F1344	S1345	S1346	R1347	Y1348	E1349	K1446	N1447	A1448	E1451	T1452	A1453	N1454	T1455	K1456	L1457	T1460	L1465	N1469	N1470	I1471	V1472	K1473	A1474	V1475	L1476	N1477	D1478																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
N1391	N1392	T1396	K1397	S1401	V1402	V1403	K1406	D1407	N1408	I1411	N1417	K1418	T1419	P1420	I1421	N1422	L1426	D1430	N1431	I1438	L1441	Q1442	D1443	F1444	S1445	K1446	N1447	A1448	E1451	T1452	A1453	N1454	T1455	K1456	L1457	T1460	L1465	N1469	N1470	I1471	V1472	K1473	A1474	V1475	L1476	N1477	D1478																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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K1622	N1623	E1634	L1641	N1646	K1655	S1663	T1664	I1665	P1666	E1667	V1668	S1669	Q1672	G1676	T1677	E1678	S1691	W1692	K1693	Y1694	T1703	L1704	P1705	E1706	E1707	A1714	N1715	I1716	T1717	T1718	S1729	S1730	G1735	D1736	R1740	N1745	H1756	Y1757	Y1761	K1762	D1765	K1766																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
E1767	N1768	K1769	E1770	L1772	V1778	Y1779	D1780	A1781	F1782	R1783	T1788	N1789	T1792	Q1793	E1794	A1795	T1799	N1800	F1807	F1808	G1809	H1817	N1818	K1819	H1820	F1829	Y1830	Y1831	M1832	L1837	S1840	T1844	Y1845	T1846	H1847	E1848	M1849	T1850	S1853	D1854	R1855	E1856	I1857	Y1858	L1859	P1870																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Y1873	A1874	K1875	G1876	L1877	N1882	S1893	V1894	L1895	D1898	D1899	S1900	E1901	R1905	L1906	Q1907	I1908	A1909	D1910	T1916	T1919	M1920	F1927	F1928	G1929	L1931	E1936	E1939	G1940	V1943	A1944	K1945	L1946	D1947	E1950	K1951	K1957	K1964	D1965	P1966	G1968	N1969	S1970	V1971	R1978	L1979	L1980	T1981																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	443908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.738	Depositor
Minimum map value	-1.169	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.43	Depositor
Map size (\AA)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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	0.20	2/10533 (0.0%)	0.45	4/14226 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	954	PRO	CG-CD	-8.68	1.21	1.50
1	A	954	PRO	N-CD	5.12	1.54	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	954	PRO	CA-N-CD	-11.39	96.05	112.00
1	A	954	PRO	N-CD-CG	-10.91	86.83	103.20
1	A	954	PRO	CA-CB-CG	-6.82	91.55	104.50
1	A	1318	VAL	N-CA-C	-5.69	106.85	111.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1055	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10350	0	10260	227	0
All	All	10350	0	10260	227	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 11.

The worst 5 of 227 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:1969:ASN:HD21	1:A:2077:ILE:HB	1.48	0.78
1:A:1204:GLY:O	1:A:1238:LYS:NZ	2.17	0.76
1:A:1655:LYS:HB3	1:A:1707:GLU:HA	1.68	0.75
1:A:1370:GLU:OE1	1:A:1378:ARG:NH1	2.20	0.74
1:A:2191:LYS:HG3	1:A:2192:ASP:H	1.54	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1293/2201 (59%)	1176 (91%)	117 (9%)	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	1148/1915 (60%)	1148 (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 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1653	GLN
1	A	2017	HIS
1	A	1715	ASN
1	A	2144	ASN
1	A	1923	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.

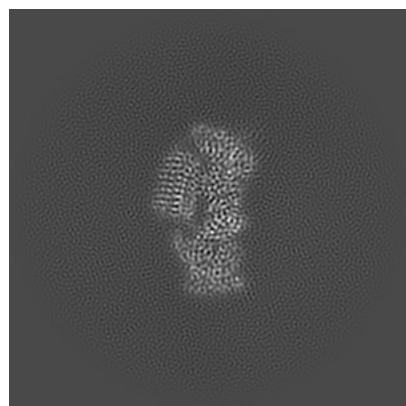
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26812. These allow visual inspection of the internal detail of the map and identification of artifacts.

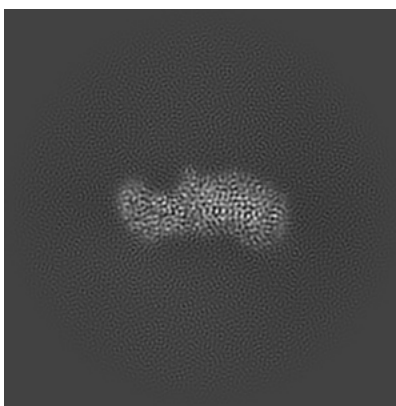
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

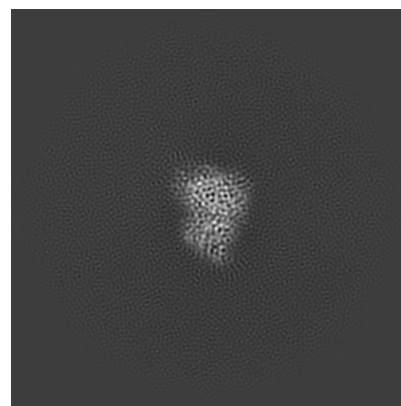
6.1.1 Primary map



X

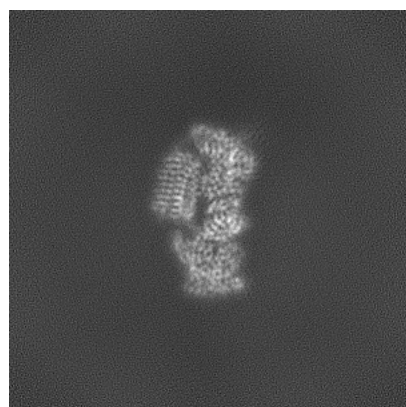


Y

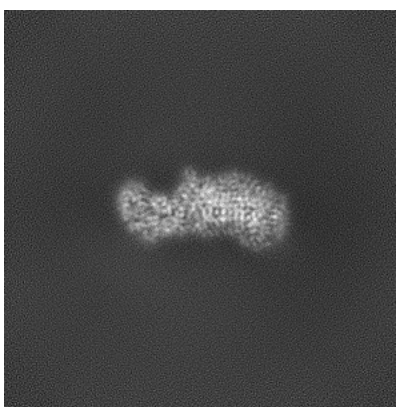


Z

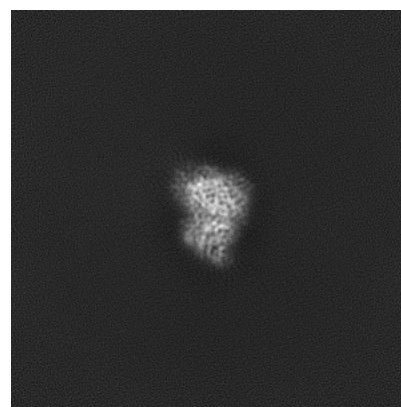
6.1.2 Raw map



X



Y

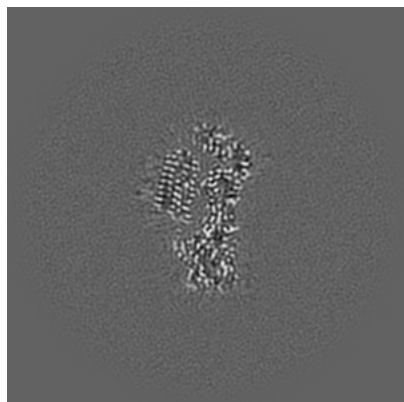


Z

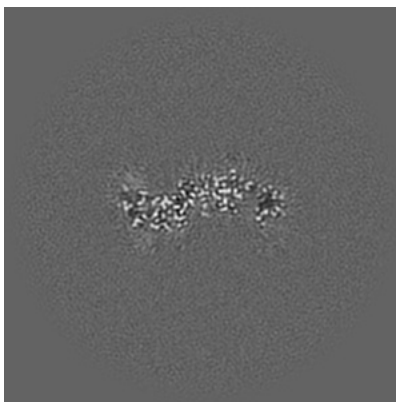
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

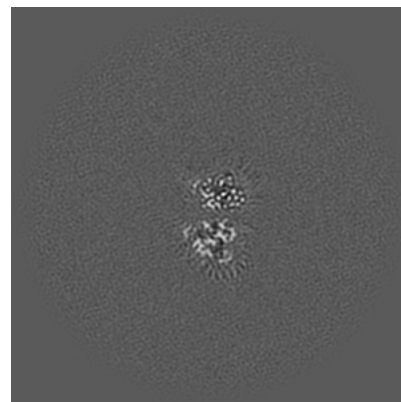
6.2.1 Primary map



X Index: 180

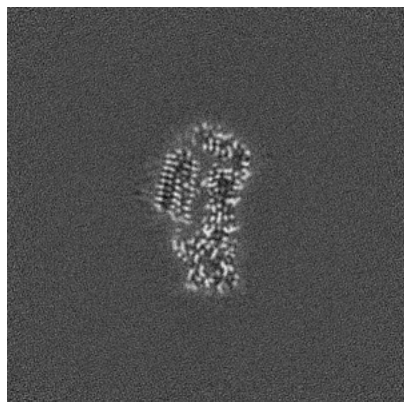


Y Index: 180

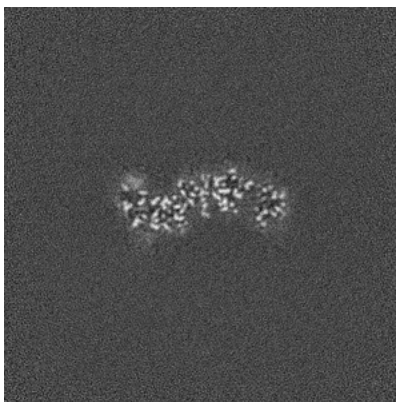


Z Index: 180

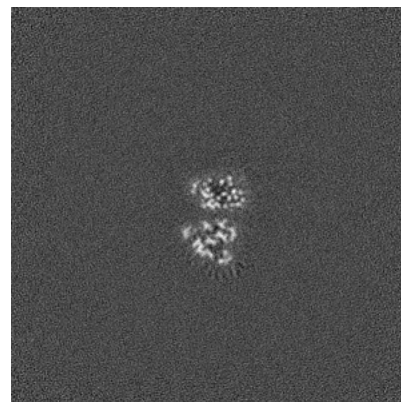
6.2.2 Raw map



X Index: 180



Y Index: 180

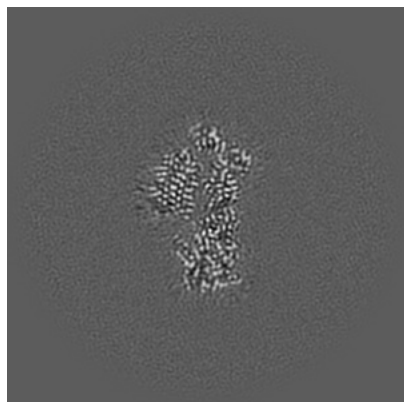


Z Index: 180

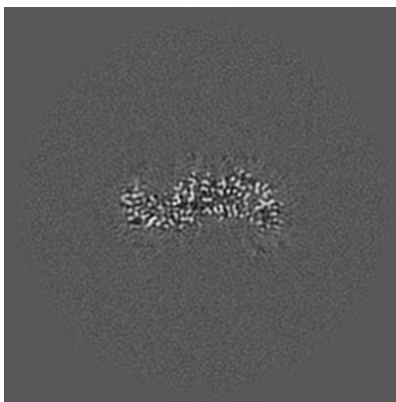
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

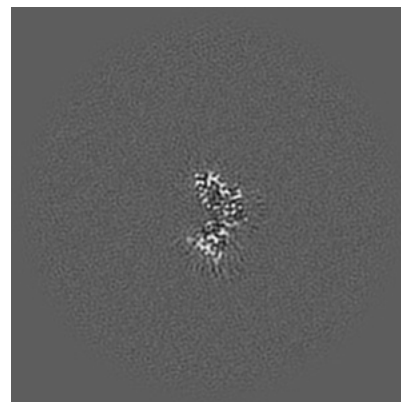
6.3.1 Primary map



X Index: 184

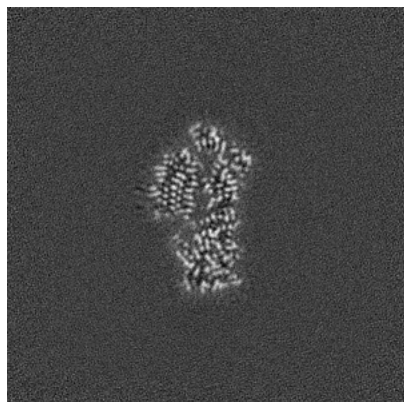


Y Index: 188

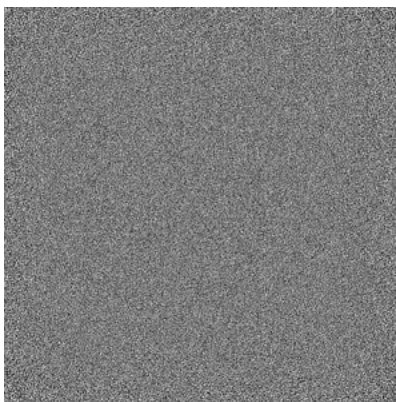


Z Index: 197

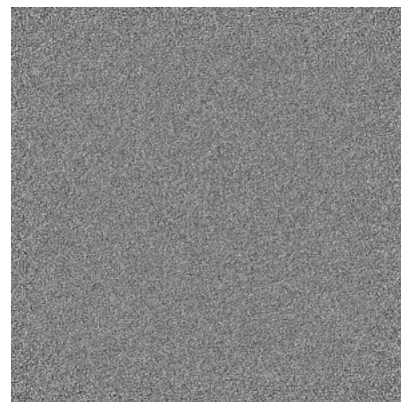
6.3.2 Raw map



X Index: 184



Y Index: 0

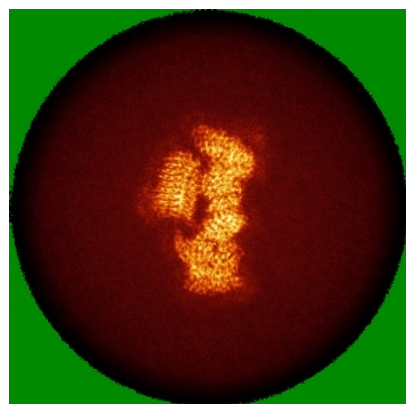


Z Index: 0

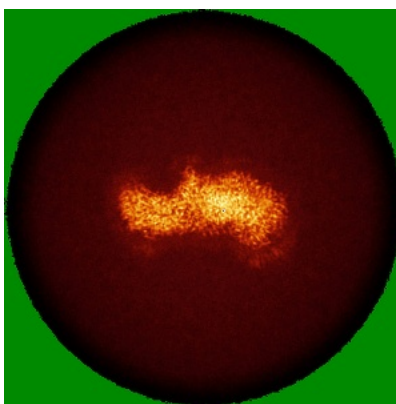
The images above show the largest variance slices of the map in three orthogonal directions.

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

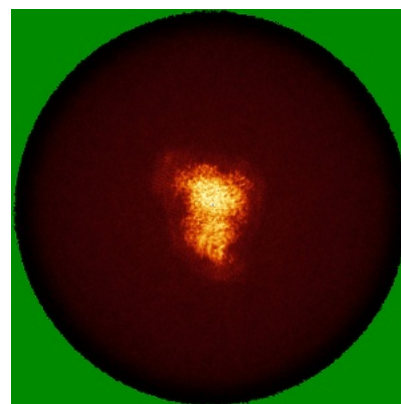
6.4.1 Primary map



X

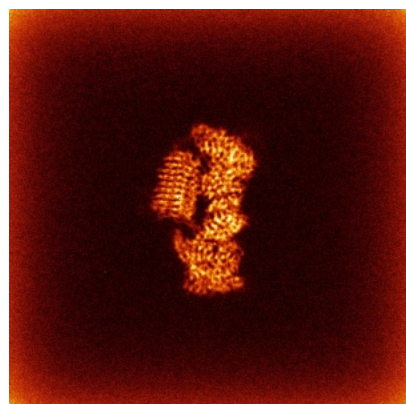


Y

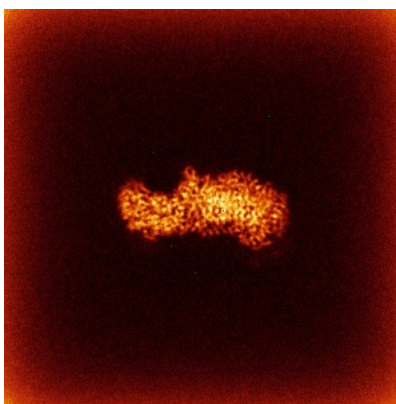


Z

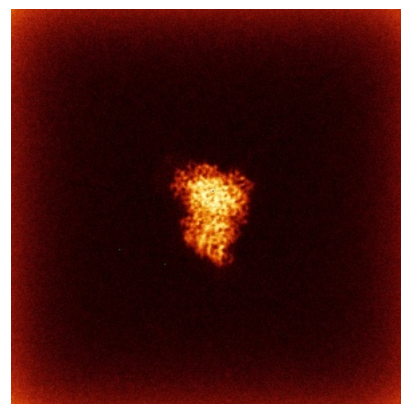
6.4.2 Raw map



X



Y

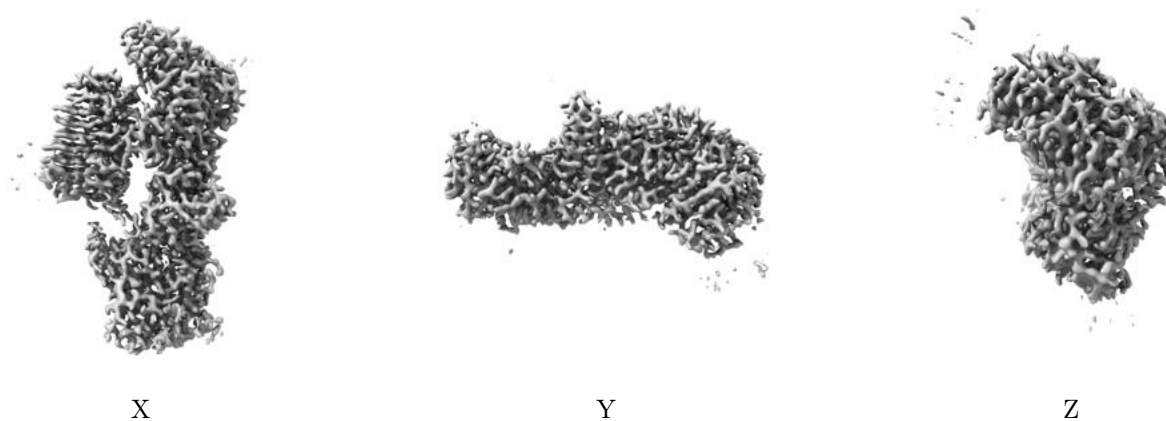


Z

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

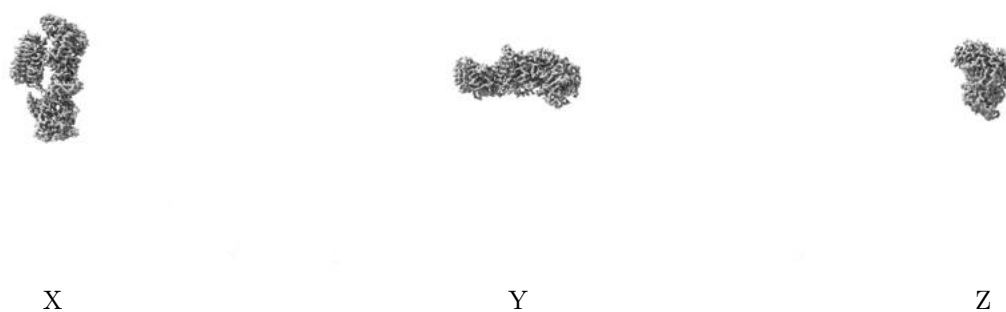
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.43. 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.

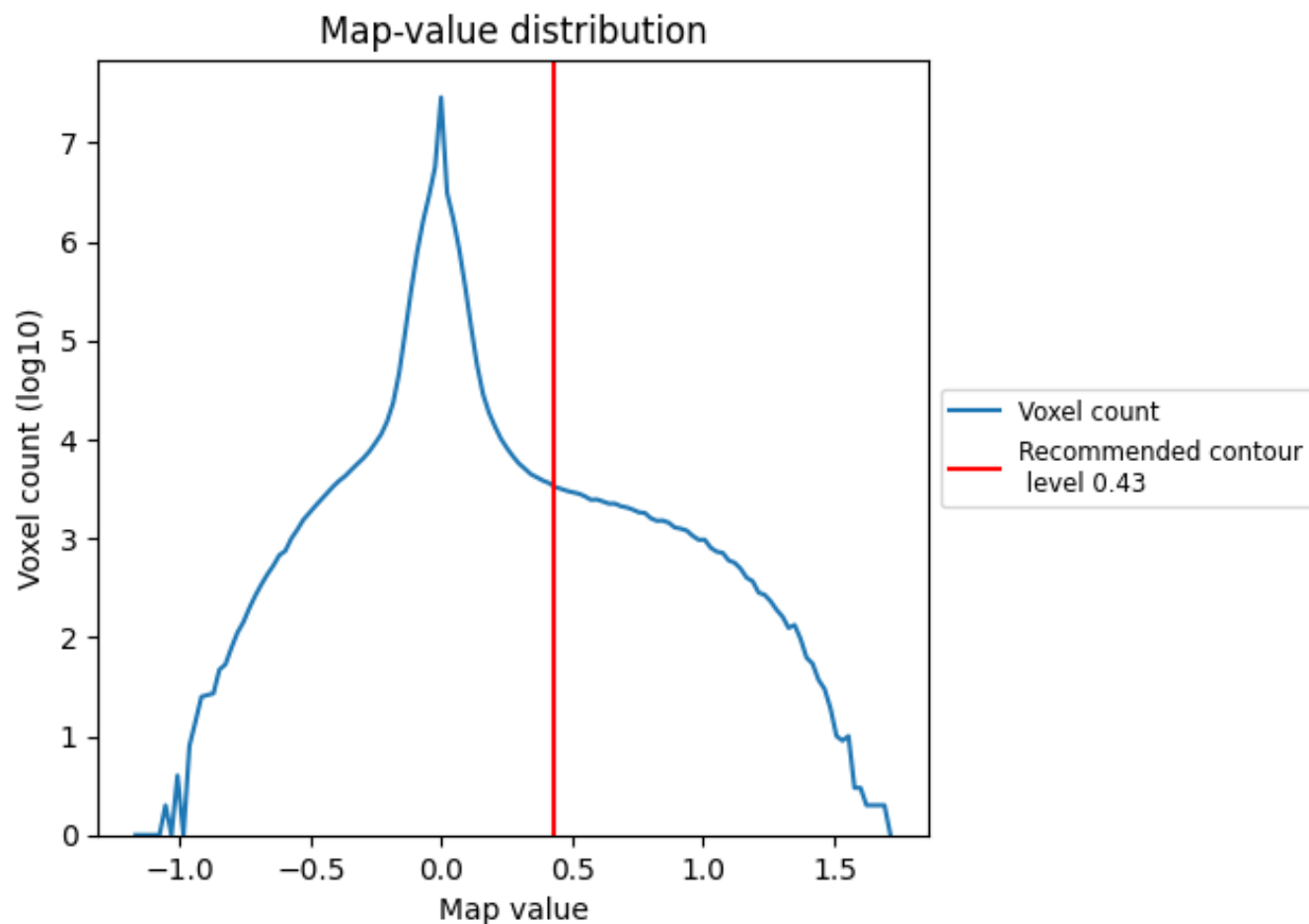
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

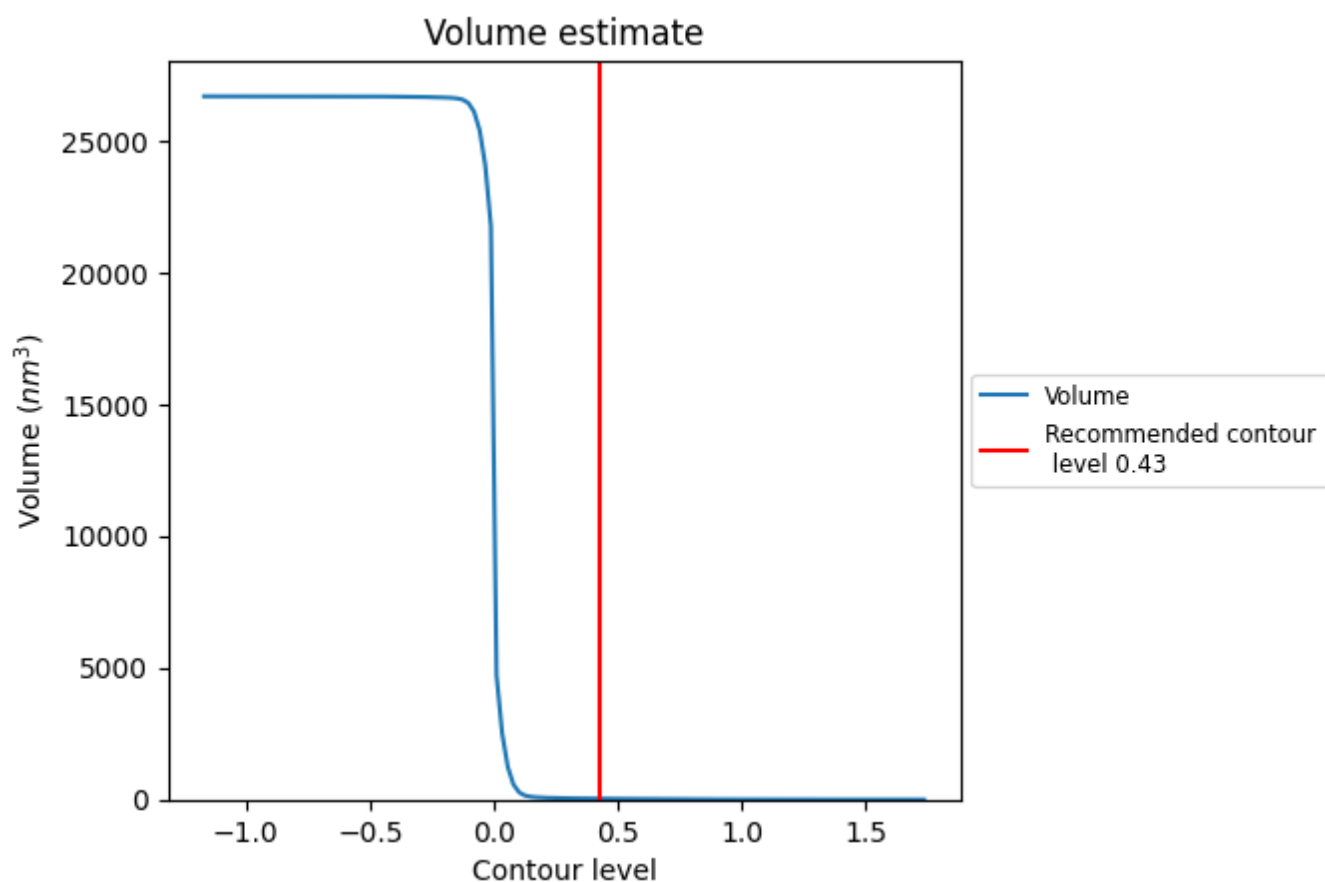
This section contains the results of statistical analysis of the map.

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.

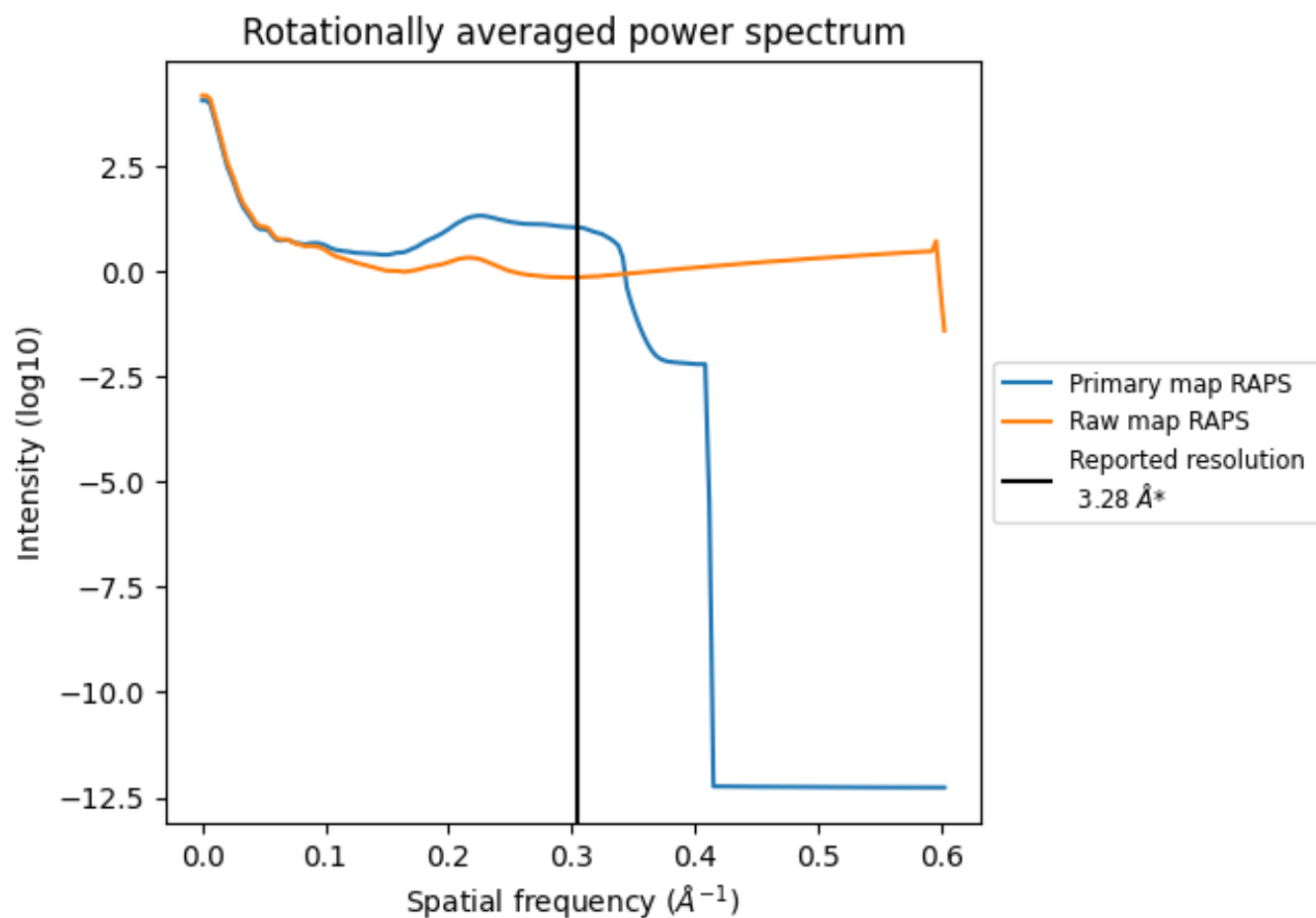
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm³; this corresponds to an approximate mass of 31 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 ⓘ

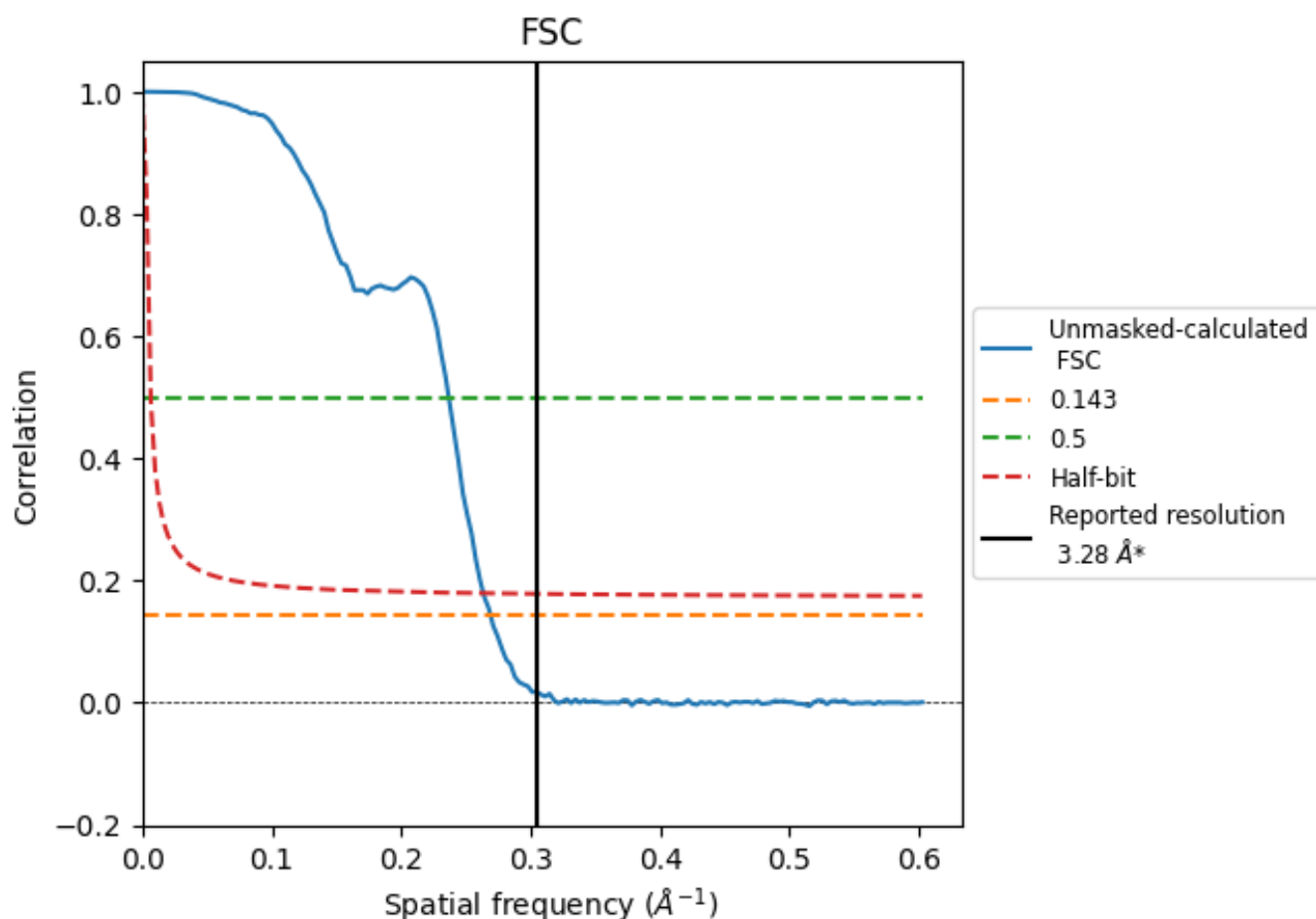


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

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 0.305 \AA^{-1}

8.2 Resolution estimates [i](#)

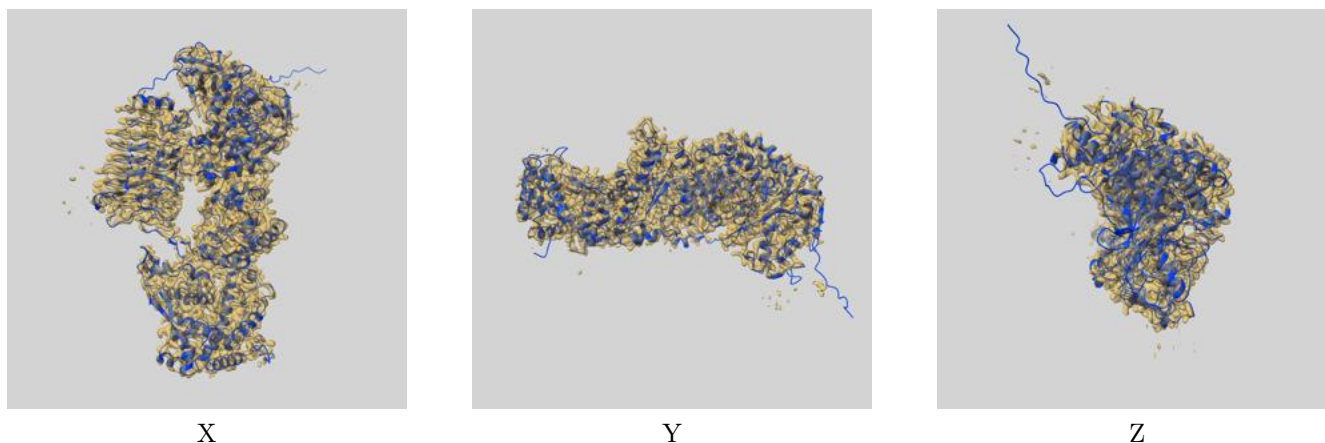
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.22	3.80

*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 3.72 differs from the reported value 3.28 by more than 10 %

9 Map-model fit [i](#)

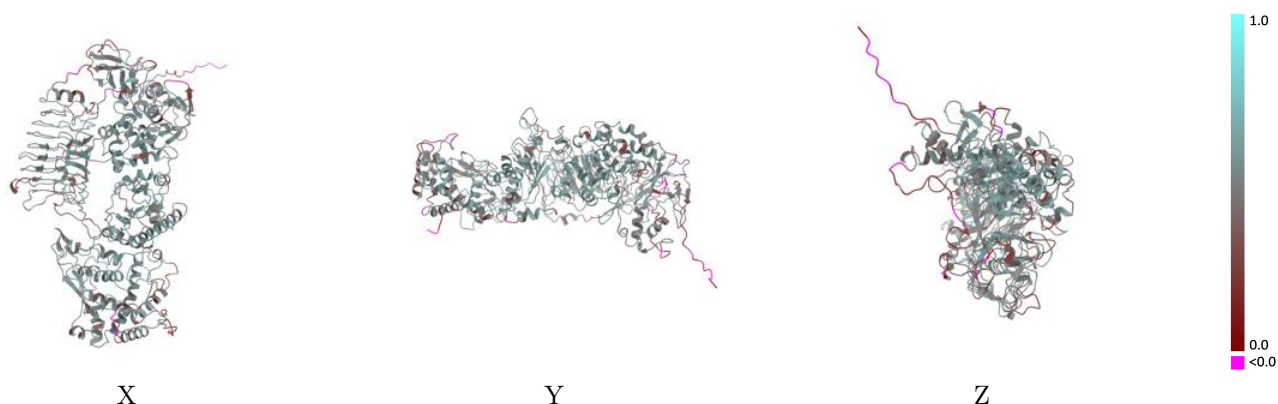
This section contains information regarding the fit between EMDB map EMD-26812 and PDB model 7UVK. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



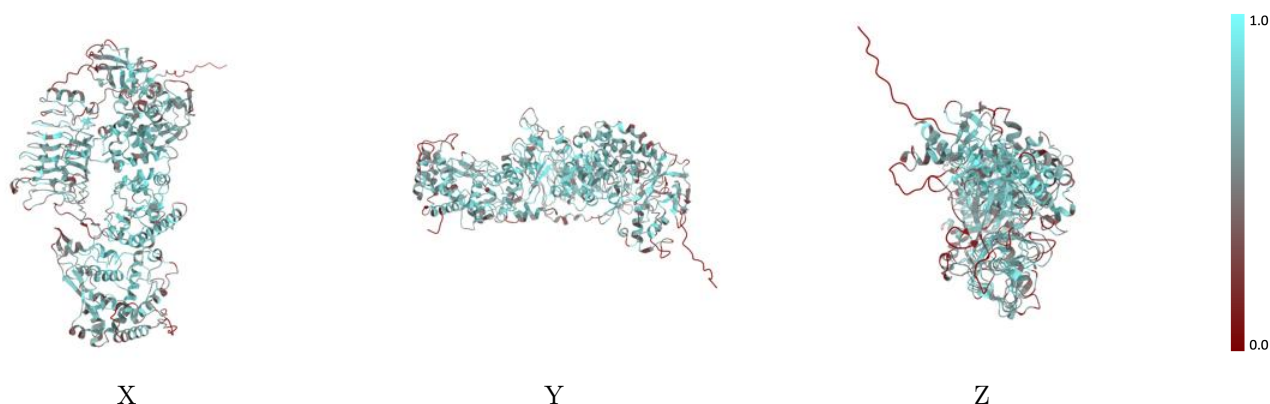
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



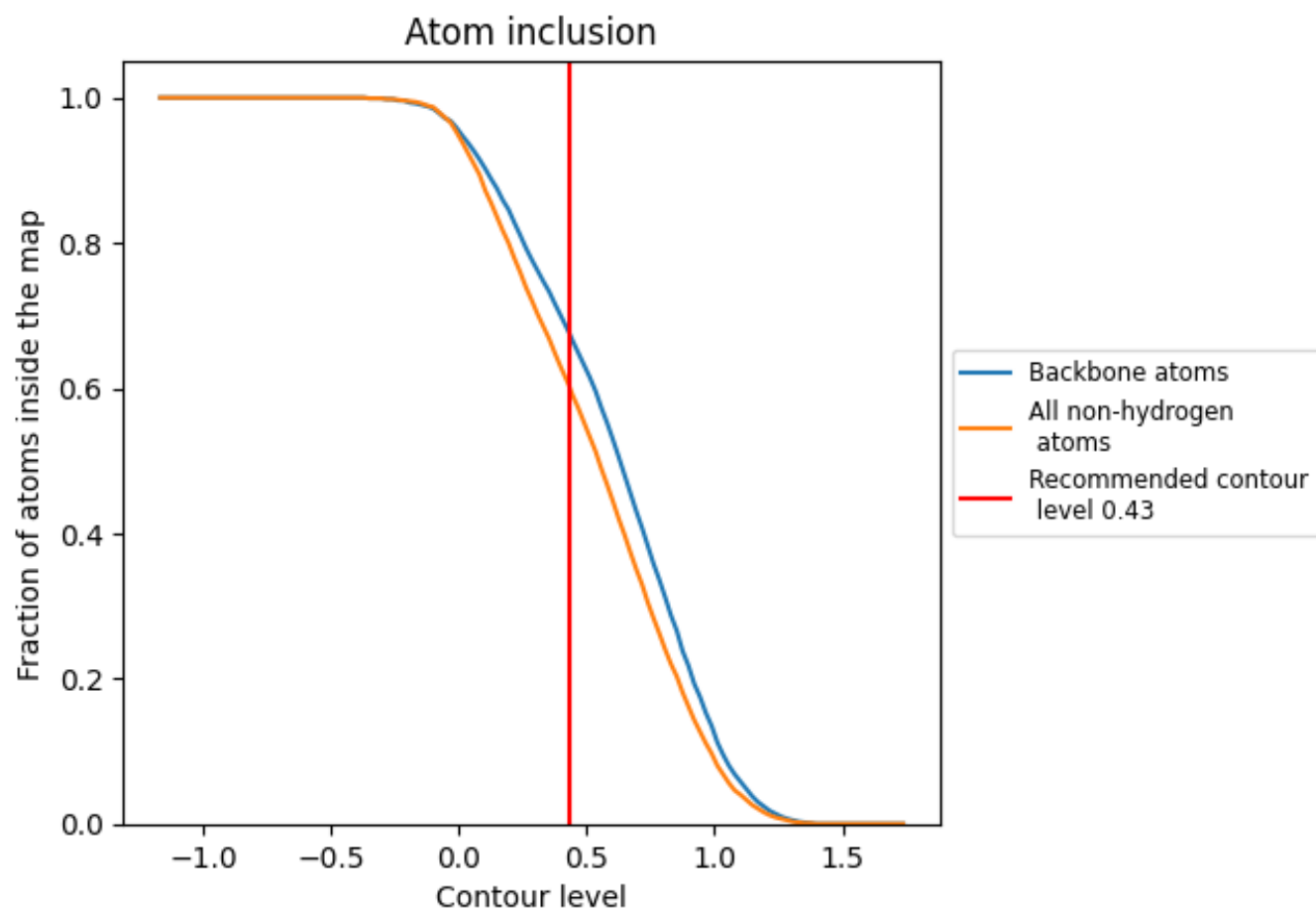
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.43).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 60% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6040	<div></div> 0.4820
A	<div></div> 0.6040	<div></div> 0.4820

