



wwPDB EM Validation Summary Report ⓘ

Feb 22, 2025 – 01:54 PM EST

PDB ID : 9EA7
EMDB ID : EMD-47801
Title : The Structure of ApoB100 from Human Low-Density Lipoprotein
Authors : Berndsen, Z.T.; Cassidy, C.K.
Deposited on : 2024-11-10
Resolution : 9.00 Å(reported)
Based on initial model : .

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.dev117
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) : 2.41.4

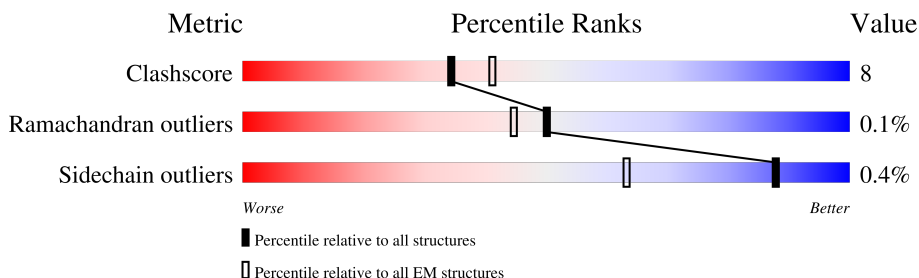
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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	4563	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 72328 atoms, of which 36245 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.

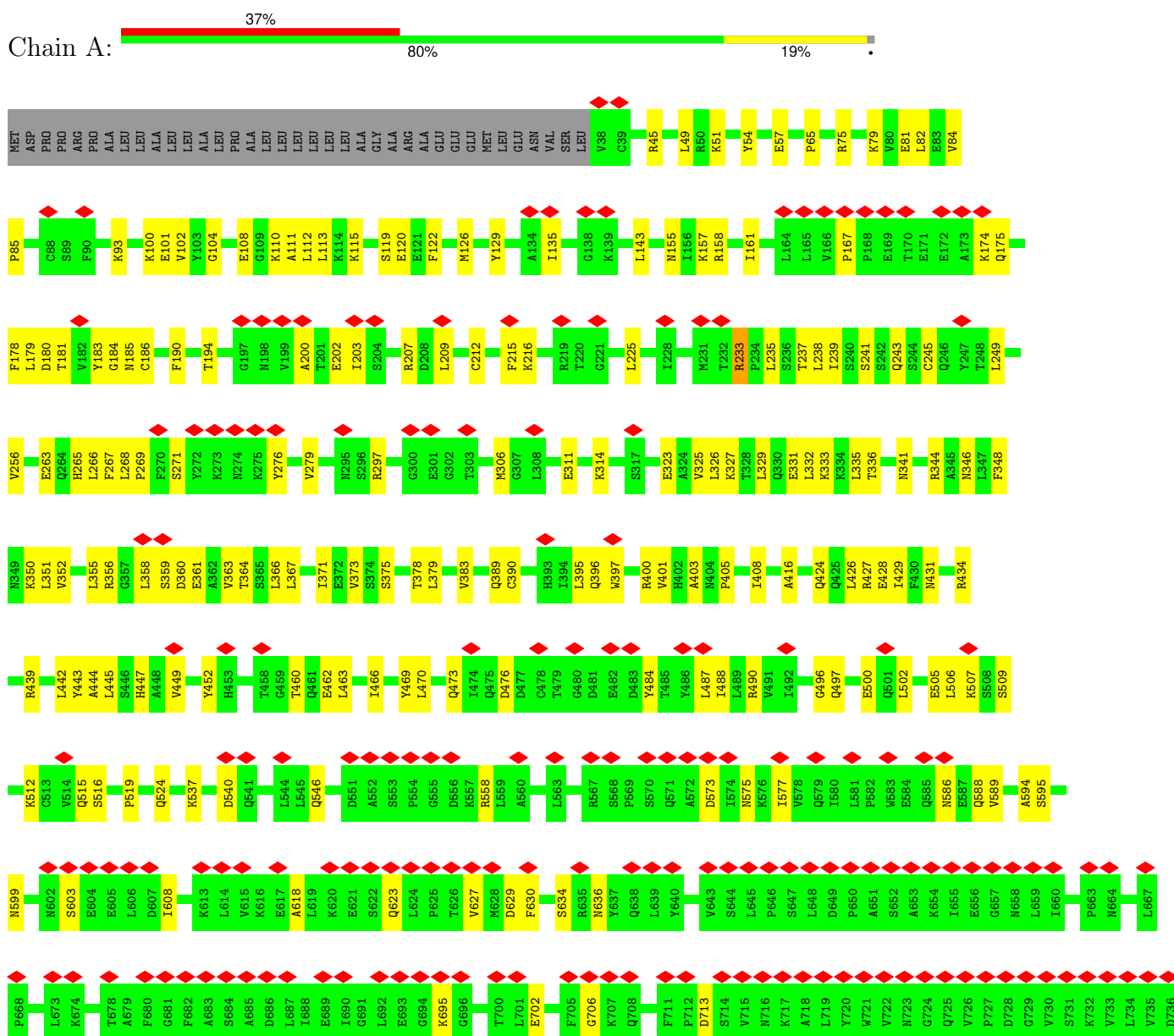
- Molecule 1 is a protein called Apolipoprotein B 100.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	4526	72328	23018	36245	6066	6897	102	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: Apolipoprotein B 100







E4181	F4182	V4186	K4187	H4188	L4189	I4190	L4193	I4194	D4195	F4196	L4197	H4198	F4199	P4200	R4201	F4202	Q4203	F4204	P4205	G4206	K4207	P4208	Q4209	G4209	I4210	Y4211	T4212	R4213	E4214	Q4215	L4216	Q4217	T4218	M4219	F4220	I4221	R4222	E4223	V4224	Q4225	T4226	V4227	L4228	V4231	Y4232	S4233	K4234	V4235	H4236	N4237	Q4238	S4239	E4240	L4241	L4242	F4243	S4244		
R4105	Q4109	E4113	W4114	Y4115	Y4116	Q4117	R4121	Q4122	I4123	D4124	D4125	I4126	D4127	W4128	R4129	F4130	K4131	T4137	Y4141	W4144	K4145	D4146	K4147	A4148	L4151	Y4152	Q4153	E4154	L4155	L4156	T4157	Q4158	E4159	Q4160	Q4161	A4062	T4068	S4069	L4070	K4071	K4076	Y4084	Y4088	H4089	W4090	E4091	L4095	T4096	S4102										
K3994	P4004	D4016	D4017	S4020	K4021	W4022	Y4026	S4027	P4028	Q4029	S4030	S4031	P4032	D4033	F4034	K4034	K4035	L4036	T4037	I4038	F4039	L4043	R4046	E4047	S4048	D4049	E4050	E4051	I4054	E4059	E4060	A4061	A4062	T4068	S4069	L4070	K4071	K4076	Y4084	Y4088	H4089	W4090	E4091	L4095	T4096	S4102													
V3876	I3877	P3878	S3879	A3882	R3886	F3887	E3888	V3889	D3890	S3891	Y3894	N3895	A3906	D3907	Y3908	V3909	E3910	T3911	D3914	S3915	F3923	L3924	E3925	Y3926	H3934	E3937	D3938	G3939	A3942	T3948	H3951	E3952	D3953	E3957	D3961	G3962	G3966	L3967	Q3968	K3979	S3980	F3983																	
Q3802	P3803	E3804	D3805	S3806	L3807	E3817	S3818	Q3819	L3820	T3826	L3827	P3828	K3829	S3830	V3831	S3832	D3833	G3834	I3835	A3836	A3837	L3838	D3839	L3840	N3841	A3842	V3843	A3844	N3845	K3846	L3847	A3848	D3849	F3850	E3851	L3852	I3855	I3856	V3857	P3858	E3859	Q3860	T3861	I3862	E3863	S3866	I3867	K3868	F3869	S3870	V3871	P3872	A3873	G3874	I3875				
V3725	L3726	A3727	D3728	K3729	F3730	L3731	L3732	P3733	K3736	L3737	N3738	D3739	L3740	S3741	S3742	V3743	L3744	V3745	V3746	K3747	P3747	T3748	F3749	H3750	V3751	P3752	F3753	T3754	D3755	L3756	Q3757	V3758	P3759	S3760	C3761	K3762	L3763	D3764	F3765	R3766	E3767	L3768	Q3769	L3770	S3777	L3781	N3782	L3783	T3784	T3785	L3786	P3787	E3788	E3793	S3801				
K3627	R3632	W3633	K3634	N3635	E3636	W3637	R3638	S3643	F3644	Q3645	S3646	E3649	L3650	S3651	K3652	Q3653	Q3654	E3655	K3656	A3657	H3658	L3659	N3674	V3679	Y3680	W3685	D3686	K3689	S3695	I3696	R3699	Q3700	H3701	F3708	T3711	K3712	N3713	P3714	N3715	G3716	Y3717	S3718	F3719	S3720	I3721	P3722	V3723	K3724											
Y3520	L3521	N3522	S3523	S3528	K3529	V3530	F3531	L3532	Q3533	D3539	N3542	N3543	L3544	K3547	E3548	N3549	F3550	W3563	E3564	Q3572	L3573	E3574	K3575	L3576	F3577	E3582	H3583	T3584	A3587	E3590	L3591	S3592	P3593	K3594	Q3595	L3599	V3600	Q3601	V3602	H3603	P3614	D3615	L3616	A3621	N3625	T3626													
K3390	R3391	H3410	N3411	T3417	T3418	K3419	N3420	A3426	T3427	N3439	K3449	S3457	M3458	K3461	Y3462	S3466	S3467	M3468	L3469	Y3470	G3475	K3480	L3481	S3482	L3483	E3484	F3490	S3491	I3492	E3493	S3494	S3495	T3496	K3497	G3498	D3499	V3500	S3506	R3507	E3508	Y3509	S3510	T3512	I3513	T3519														
H3239	D3240	E3241	L3242	R3243	R3244	T3245	F3246	K3247	I3248	P3249	G3250	F3251	T3252	V3253	P3254	V3255	V3256	N3257	V3258	E3259	V3260	S3261	P3262	F3263	T3264	I3265	E3266	M3267	S3268	A3269	F3270	G3271	P3272	V3273	F3274	P3275	K3276	A3277	V3278	S3279	M3280	P3281	S3282	F3283	S3284	I3285	L3286	G3287	S3288	D3289	V3290	S3291	V3292	P3293	S3294	T3295	L3296	I3297	S3298
K3178	K3179	N3180	R3183	H3184	S3185	I3186	T3187	N3188	P3189	L3190	A3191	V3192	L3193	C3194	E3195	F3196	I3197	S3198	Q3199	S3200	I3201	K3202	S3203	F3204	R3205	R3206	H3207	F3208	E3209	K3210	N3211	R3212	N3213	N3214	A3215	L3216	L3217	F3218	V3219	T3220	K3221	S3222	Y3223	N3224	E3225	F3226	K3227	I3228	K3229	F3230	D3231	K3232	K3234	A3235	E3236	K3237	S3238		
F3093	F3102	N3106	N3107	N3108	N3109	N3110	N3111	N3112	N3113	N3114	F3125	F3126	F3127	F3128	F3129	F3130	F3131	F3132	F3133	F3134	F3135	F3136	F3137	F3138	F3139	F3140	F3141	F3142	F3143	T3144	F3145	F3146	F3147	F3148	D3149	F3150	S3151	L3152	F3153	E3154	K3155	L3158	K3159	F3160	F3161	F3162	K3163	T3164	T3165	K3166	Q3167	S3168	F3169	Y3177					

Y4245	F4246	Q4247	D4248	L4249	V4250	I4251	T4252	L4253	P4254	F4255	E4256	L4257	R4258	K4259	H4260	K4261	L4262	I4263	D4264	S4267	M4268	Y4269	R4270	E4271	L4272	L4273	K4274	D4275	L4276	S4277	K4278	E4279	A4280	Q4281	E4282	V4283	F4284	K4285	A4286	I4287	Q4288	S4289	L4290	K4291	T4292	T4293	E4294	V4295	L4296	R4297	H4298	L4299	Q4300	D4301	L4302	L4303	D4304	F4305																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
		L4309	I4310																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52843	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.148	Depositor
Minimum map value	-0.560	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	490.5, 490.5, 490.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	0.25	0/36813	0.46	0/49814

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2820	ASN	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	36083	36245	36243	573	0
All	All	36083	36245	36243	573	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 573 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:500:GLU:OE2	1:A:537:LYS:NZ	1.96	0.98
1:A:325:VAL:HG13	1:A:351:LEU:HD11	1.46	0.95
1:A:323:GLU:OE1	1:A:327:LYS:NZ	2.03	0.92
1:A:3632:ARG:NH1	1:A:3633:TRP:O	2.03	0.92
1:A:3482:SER:OG	1:A:3484:GLU:OE2	1.90	0.89

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	4524/4563 (99%)	4338 (96%)	182 (4%)	4 (0%)	48 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3828	PRO
1	A	1477	GLN
1	A	3906	ALA
1	A	1804	ASN

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	4051/4080 (99%)	4033 (100%)	18 (0%)	89 91

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3638	ARG
1	A	4412	LYS
1	A	4071	LYS
1	A	2251	ASN
1	A	3389	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3051	ASN
1	A	3207	HIS
1	A	3224	ASN
1	A	1013	GLN
1	A	255	HIS

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 ⓘ

There are no chain breaks in this entry.

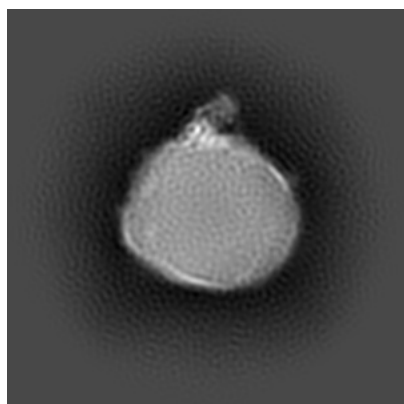
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47801. These allow visual inspection of the internal detail of the map and identification of artifacts.

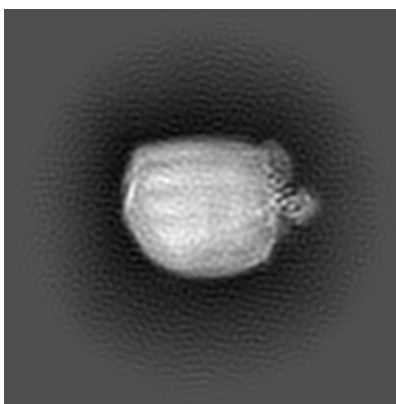
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

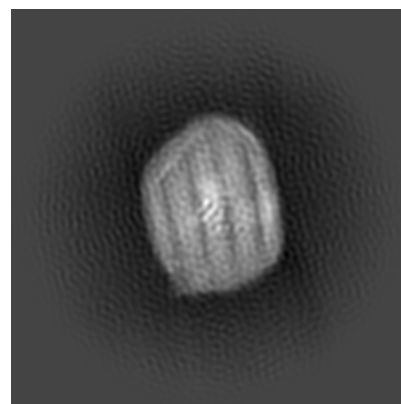
6.1.1 Primary map



X

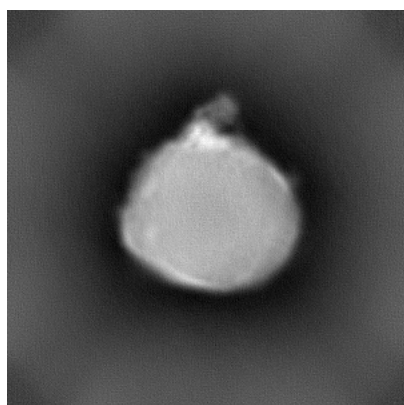


Y

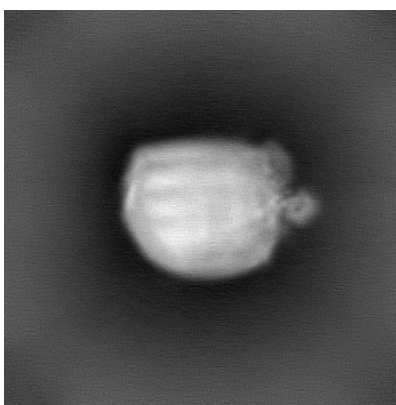


Z

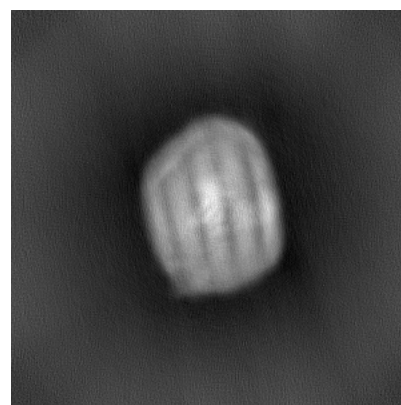
6.1.2 Raw map



X



Y

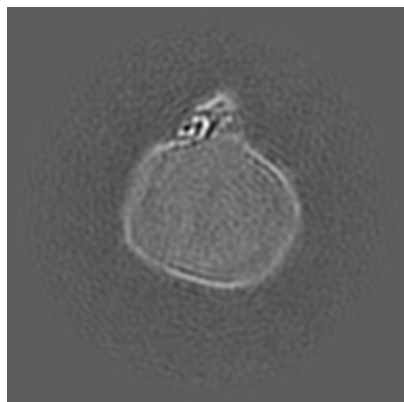


Z

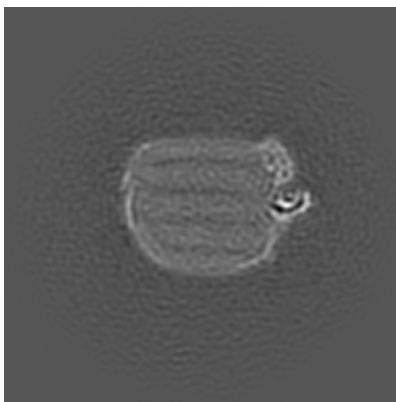
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

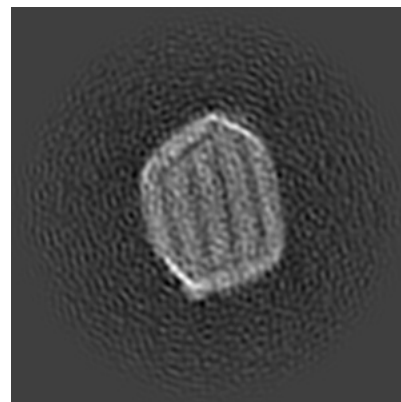
6.2.1 Primary map



X Index: 225

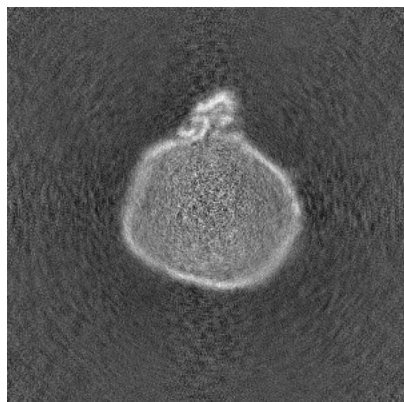


Y Index: 225

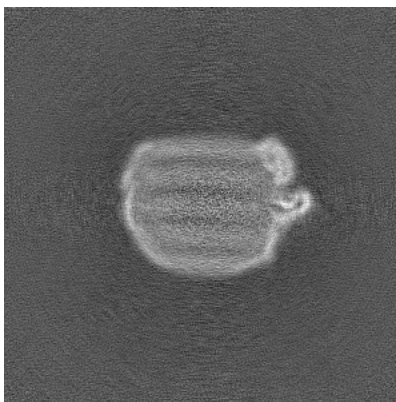


Z Index: 225

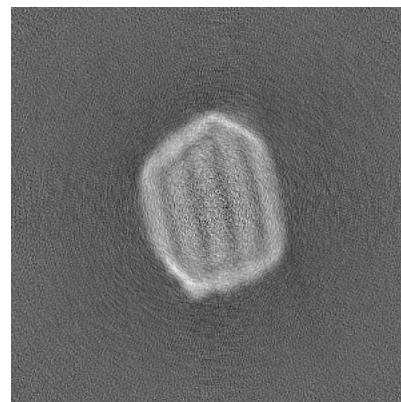
6.2.2 Raw map



X Index: 225



Y Index: 225

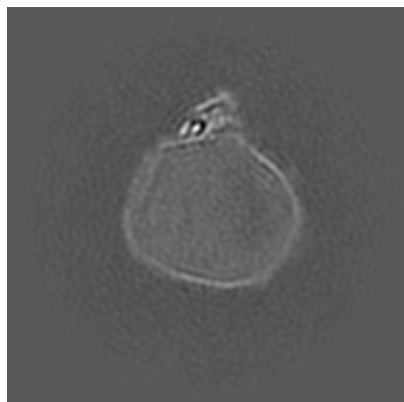


Z Index: 225

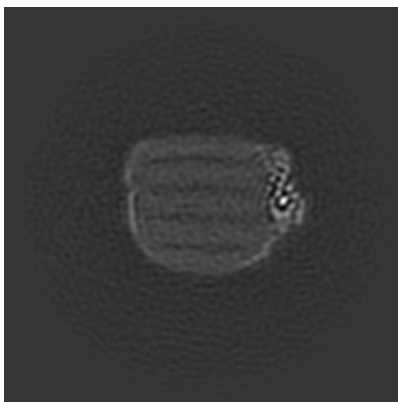
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

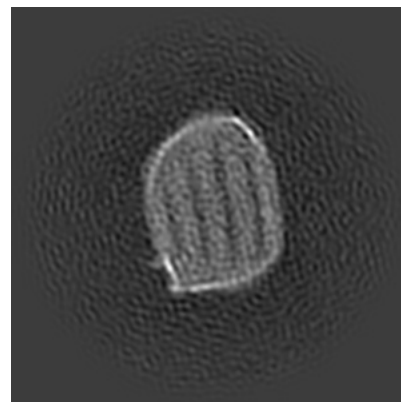
6.3.1 Primary map



X Index: 230



Y Index: 213

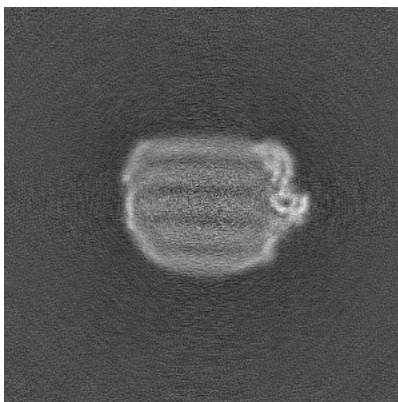


Z Index: 196

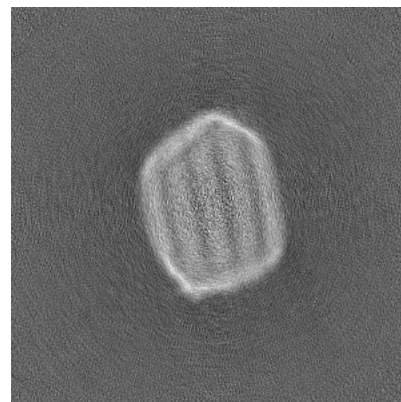
6.3.2 Raw map



X Index: 227



Y Index: 219

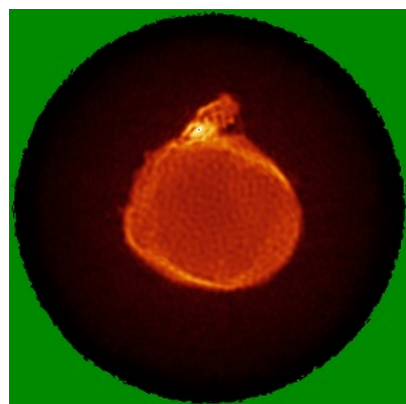


Z Index: 219

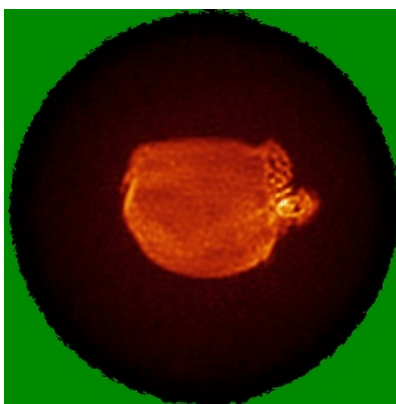
The images above show the largest variance slices of the map in three orthogonal directions.

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

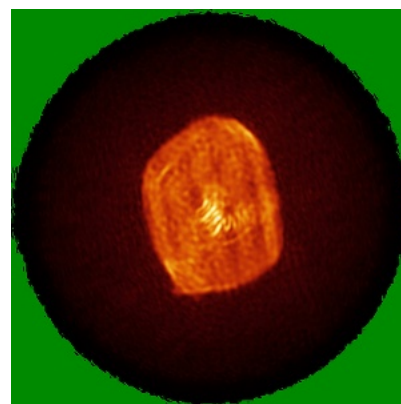
6.4.1 Primary map



X

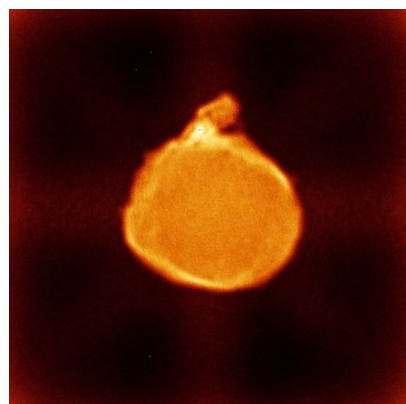


Y

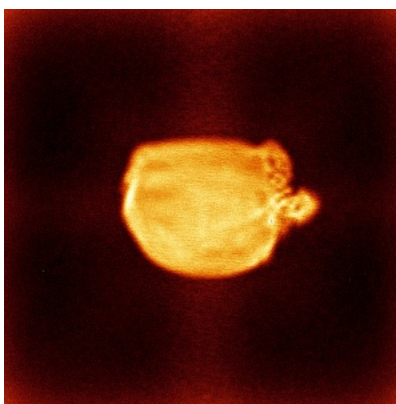


Z

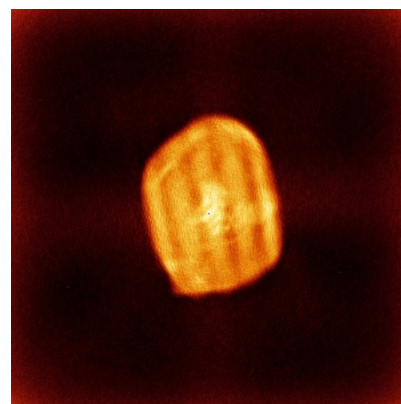
6.4.2 Raw map



X



Y

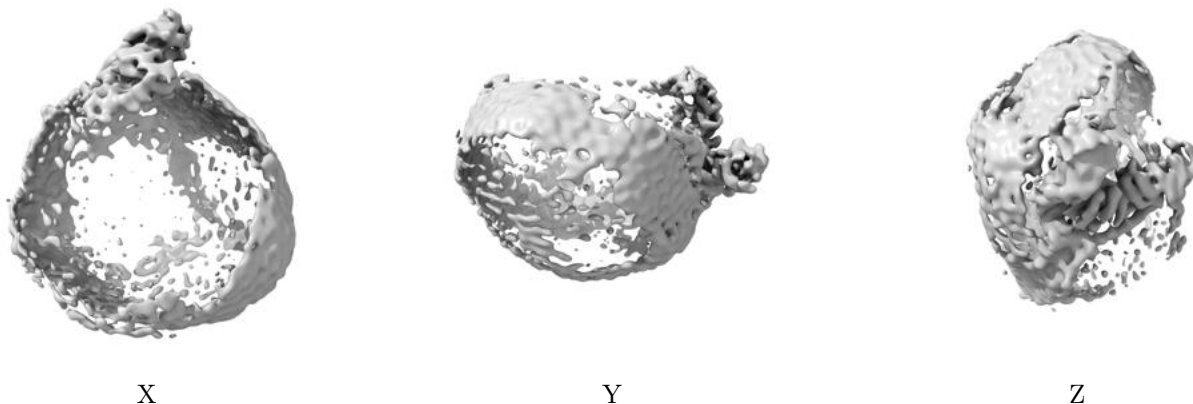


Z

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.

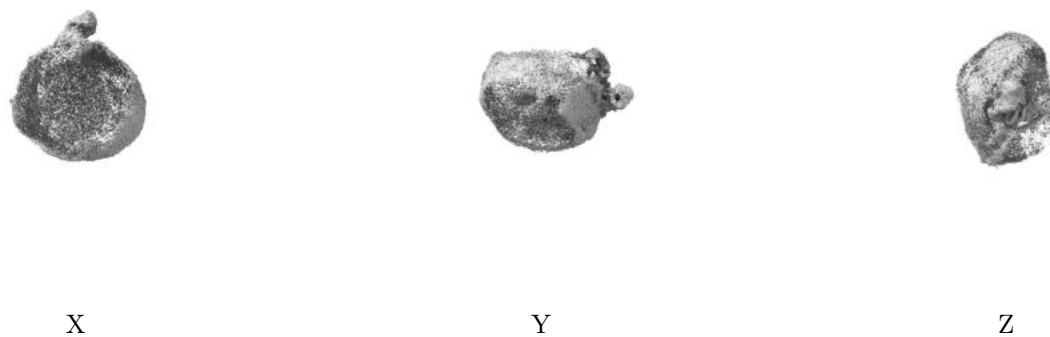
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.182. 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.

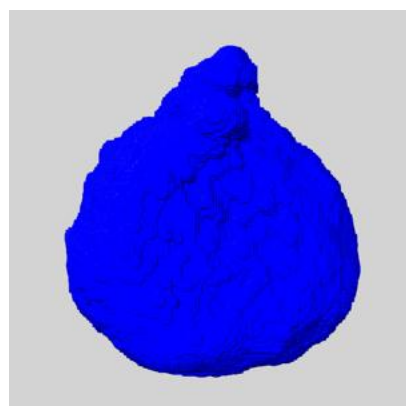
6.6 Mask visualisation [i](#)

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

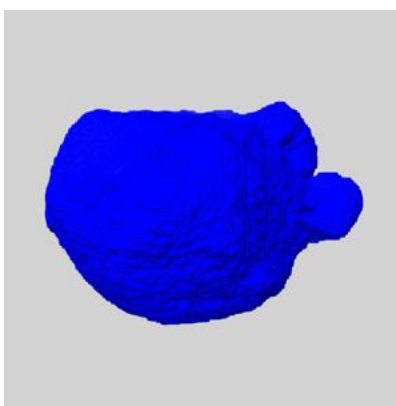
A mask typically either:

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

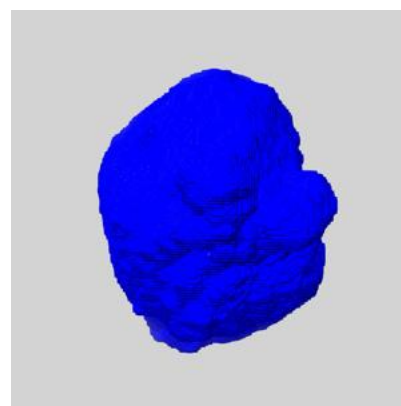
6.6.1 emd_47801_msk_1.map [i](#)



X



Y

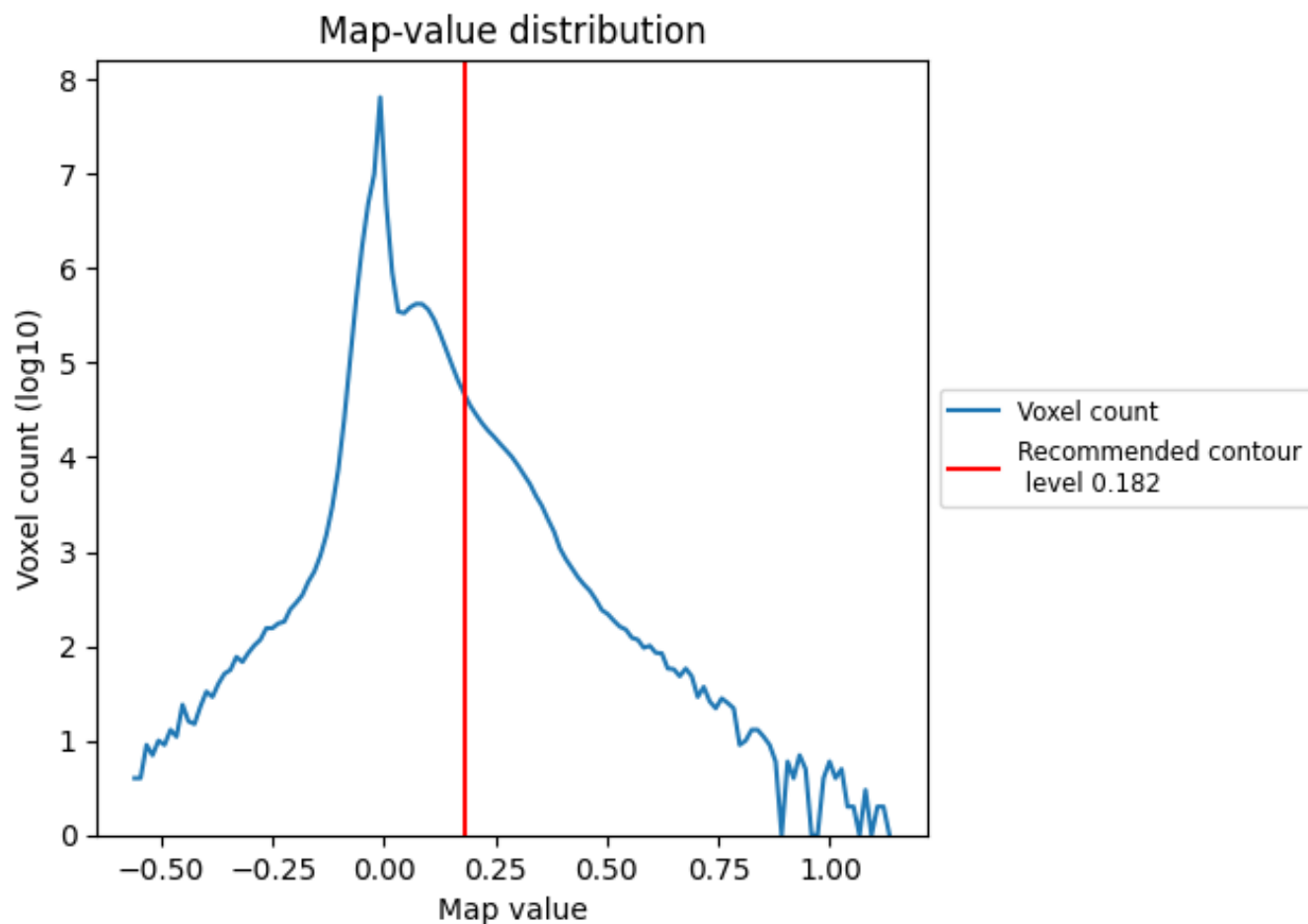


Z

7 Map analysis [i](#)

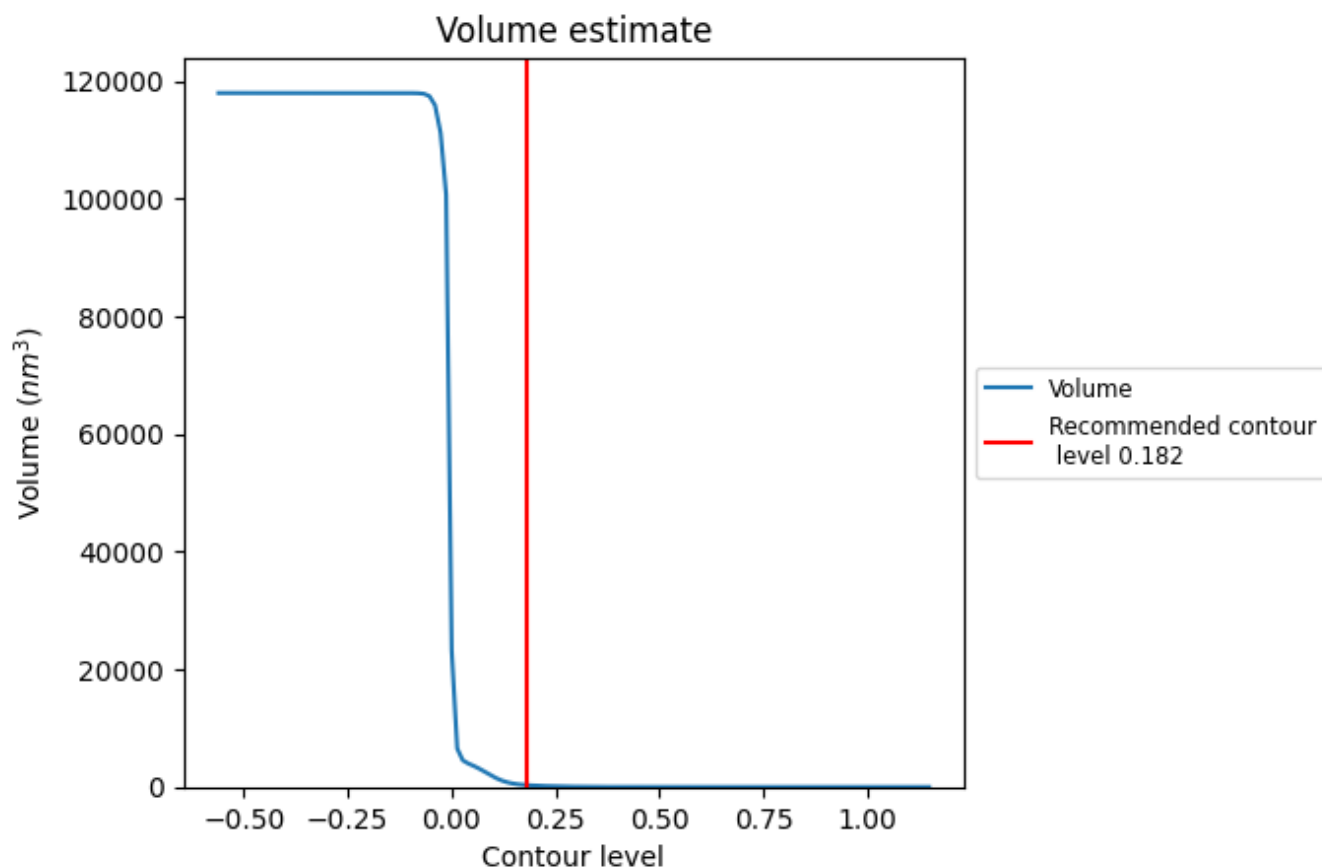
This section contains the results of statistical analysis of the map.

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.

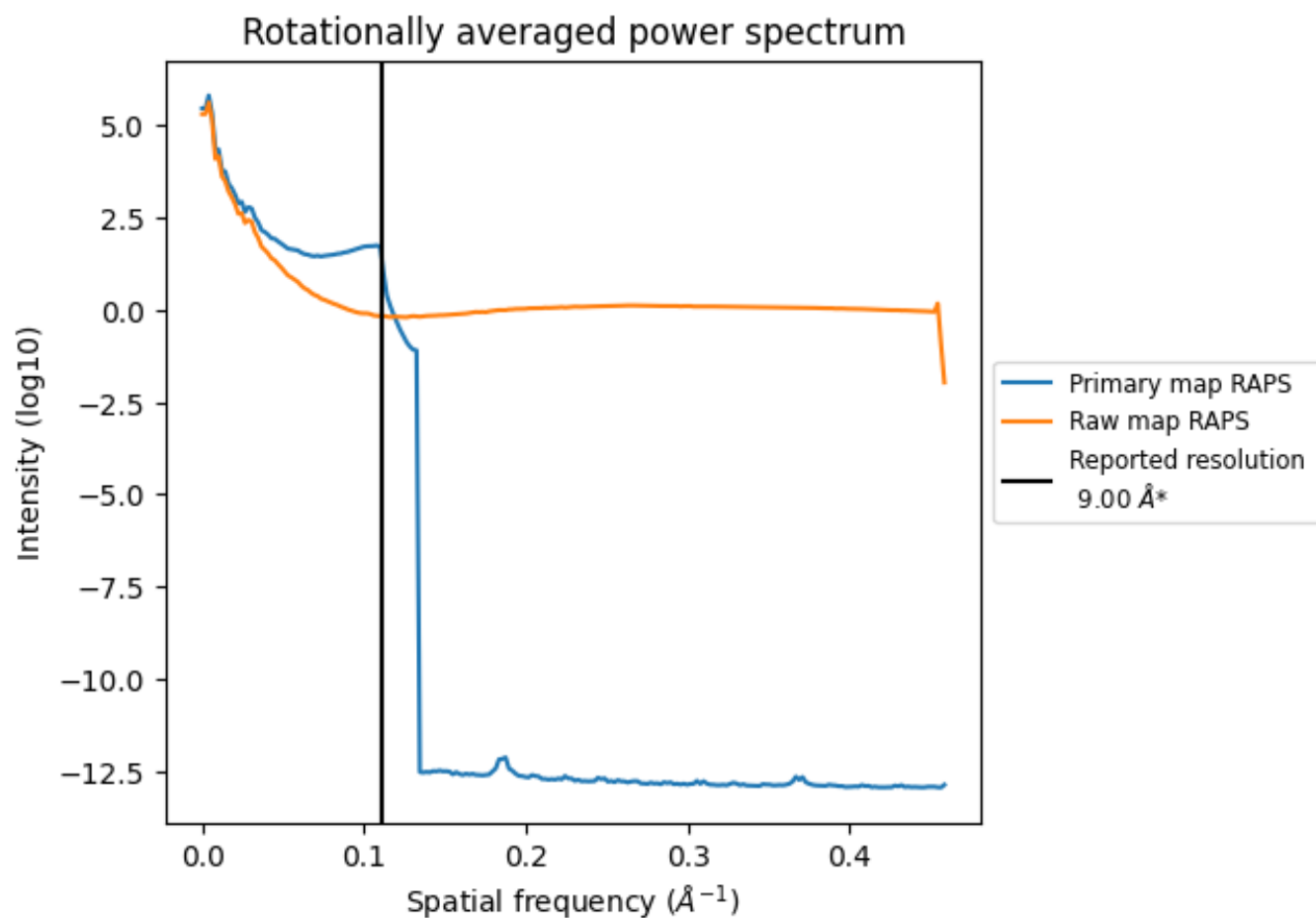
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 275 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 ⓘ

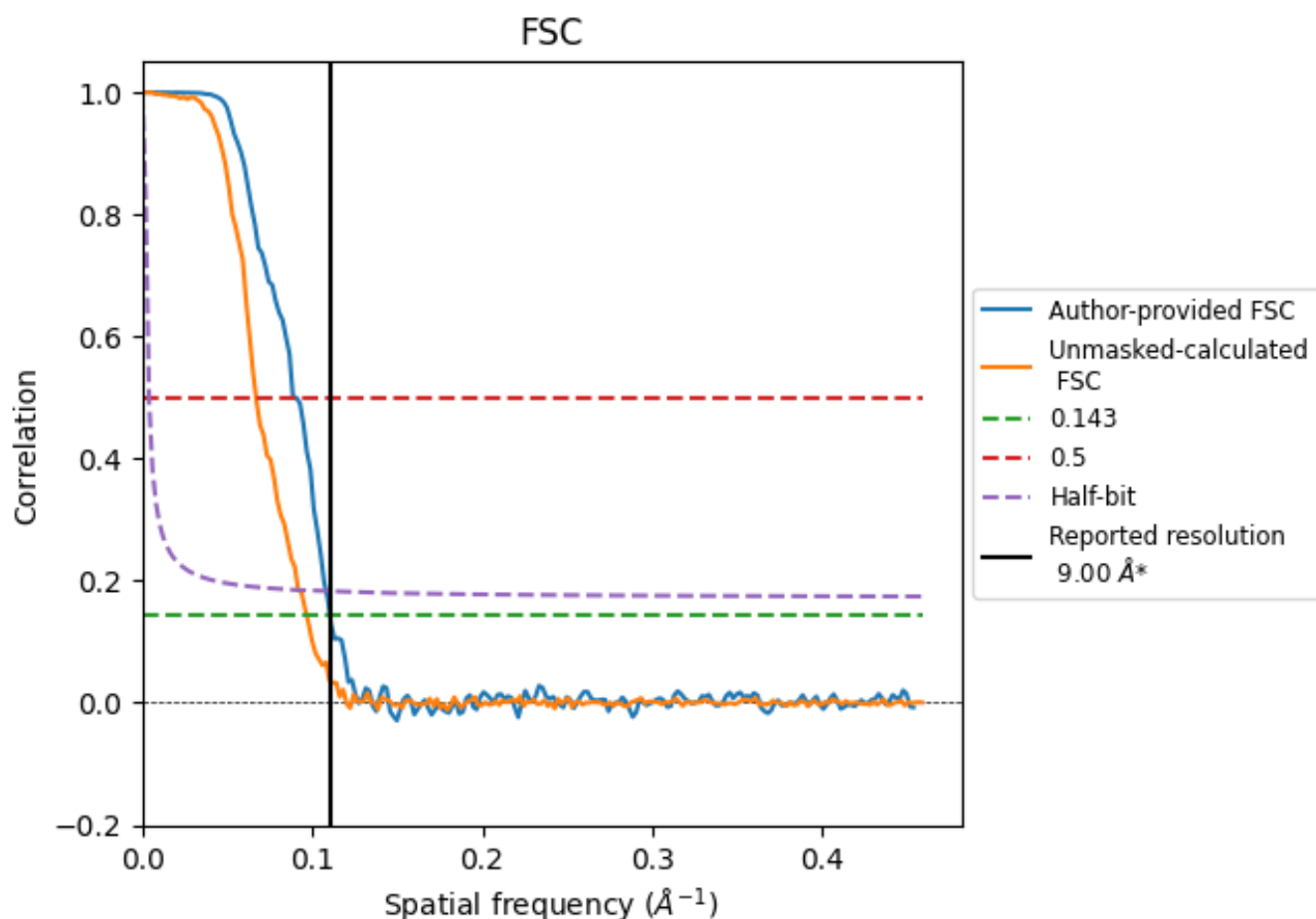


*Reported resolution corresponds to spatial frequency of 0.111 Å⁻¹

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 0.111 \AA^{-1}

8.2 Resolution estimates [i](#)

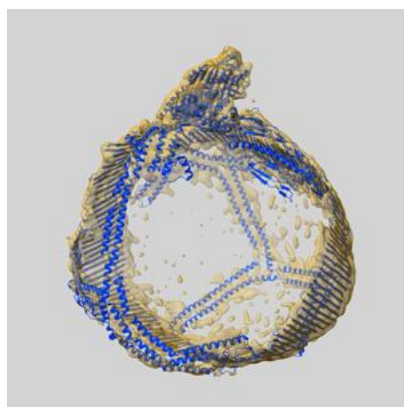
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.00	-	-
Author-provided FSC curve	9.06	11.27	9.24
Unmasked-calculated*	10.34	14.93	10.85

*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 10.34 differs from the reported value 9.0 by more than 10 %

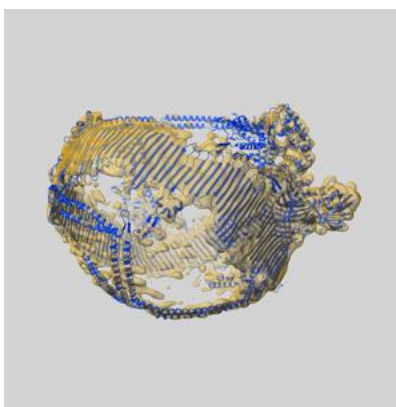
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47801 and PDB model 9EA7. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

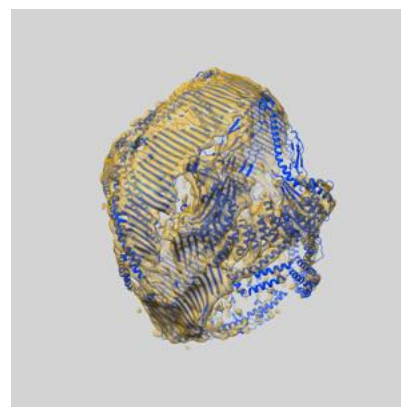
9.1 Map-model overlay [i](#)



X



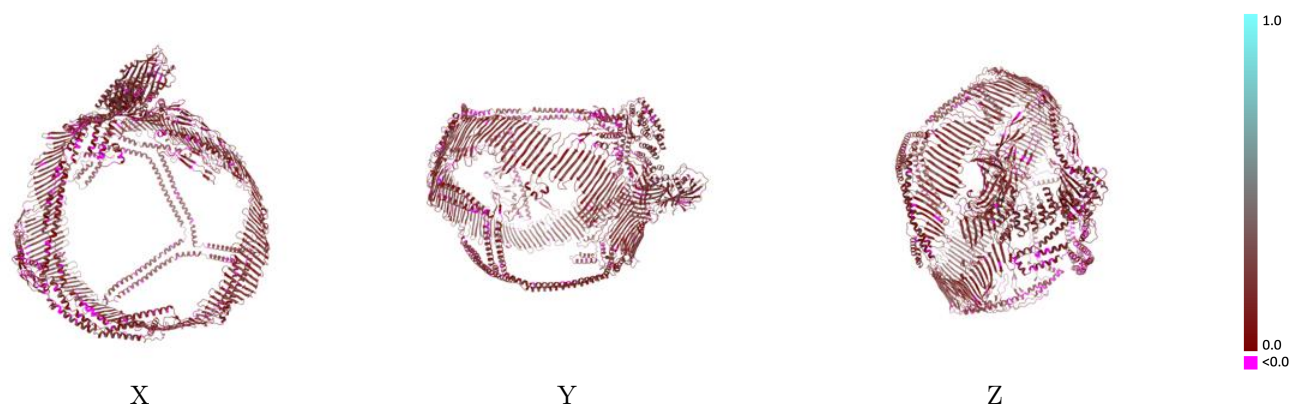
Y



Z

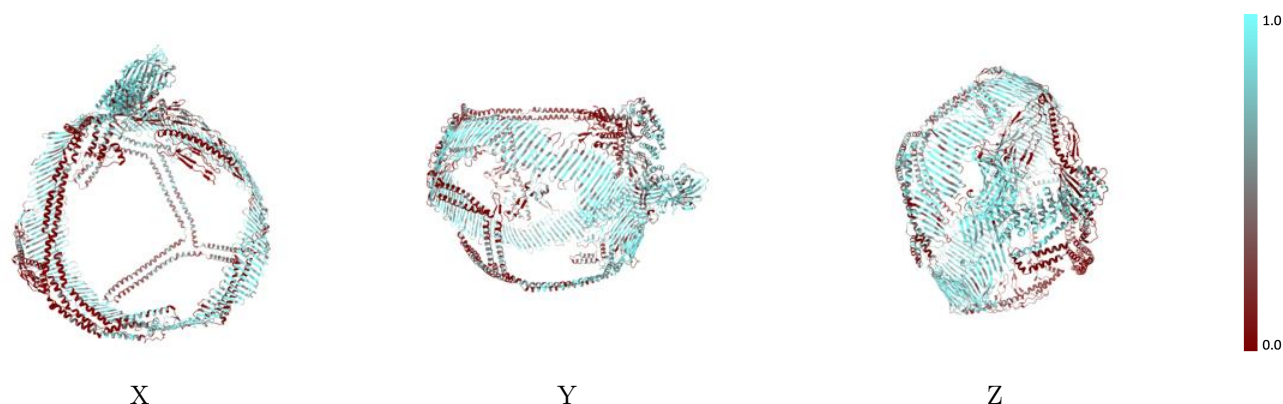
The images above show the 3D surface view of the map at the recommended contour level 0.182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



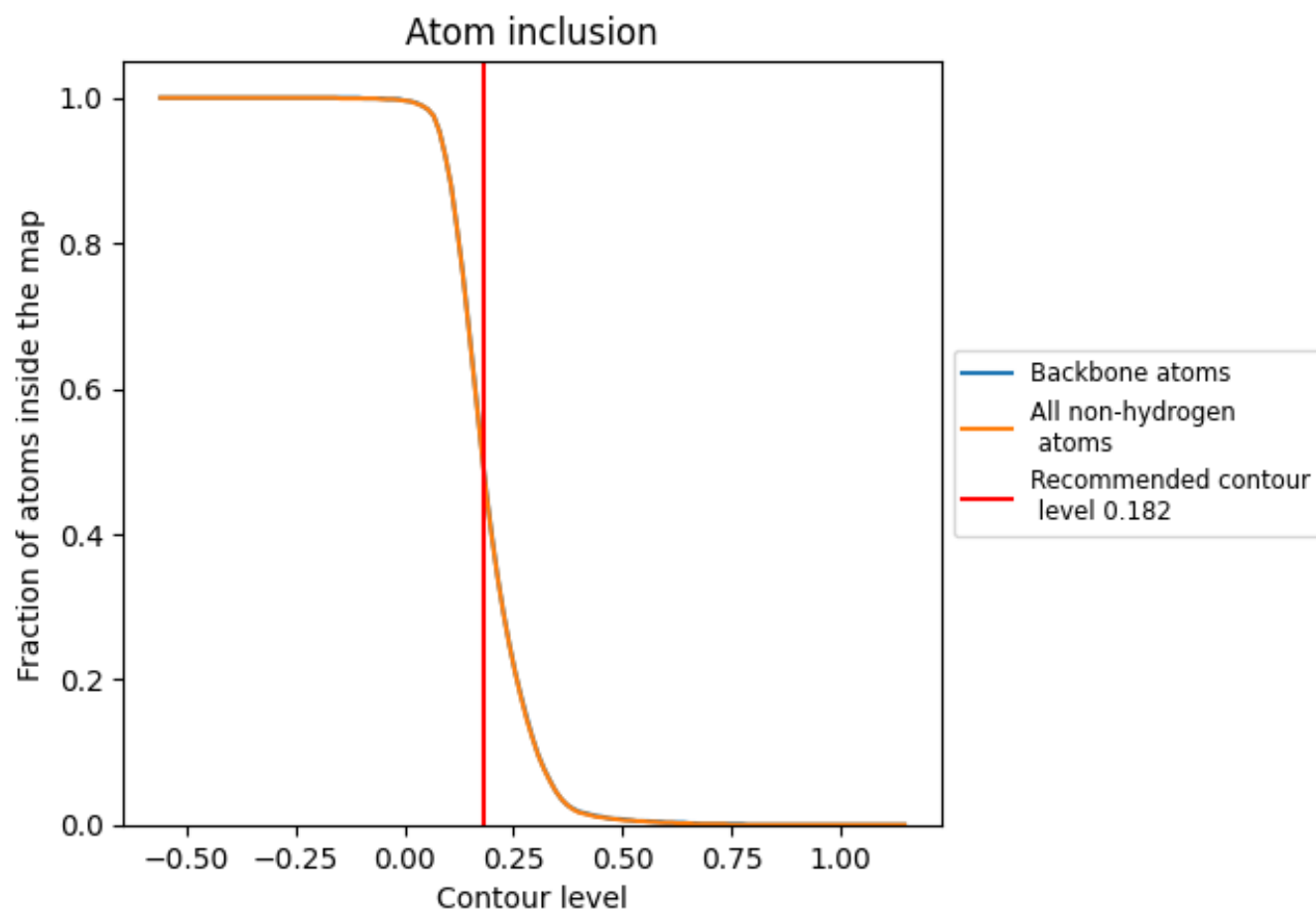
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.182).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 49% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4860	<div></div> 0.1580
A	<div></div> 0.4930	<div></div> 0.1580

