



wwPDB EM Validation Summary Report ⓘ

May 6, 2024 – 01:38 PM EDT

PDB ID : 7JQ9
EMDB ID : EMD-22427
Title : Cryo-EM structure of human HUWE1
Authors : Hunkeler, M.; Fischer, E.S.
Deposited on : 2020-08-10
Resolution : 3.10 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

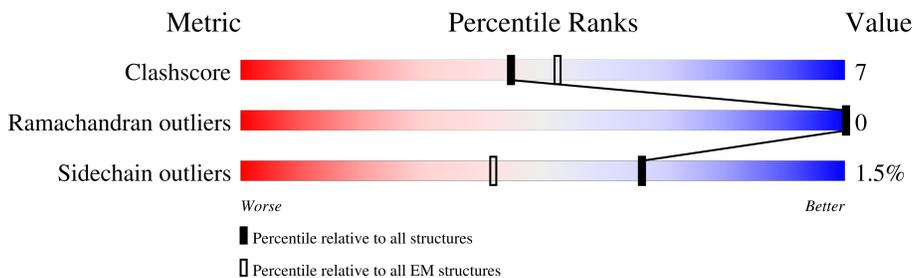
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	4411	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38719 atoms, of which 19554 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 E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	2427	38719	12225	19554	3292	3528	120	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	MET	-	expression tag	UNP Q7Z6Z7
A	-35	ASP	-	expression tag	UNP Q7Z6Z7
A	-34	TYR	-	expression tag	UNP Q7Z6Z7
A	-33	LYS	-	expression tag	UNP Q7Z6Z7
A	-32	ASP	-	expression tag	UNP Q7Z6Z7
A	-31	ASP	-	expression tag	UNP Q7Z6Z7
A	-30	ASP	-	expression tag	UNP Q7Z6Z7
A	-29	ASP	-	expression tag	UNP Q7Z6Z7
A	-28	LYS	-	expression tag	UNP Q7Z6Z7
A	-27	LEU	-	expression tag	UNP Q7Z6Z7
A	-26	ALA	-	expression tag	UNP Q7Z6Z7
A	-25	ALA	-	expression tag	UNP Q7Z6Z7
A	-24	ALA	-	expression tag	UNP Q7Z6Z7
A	-23	ASN	-	expression tag	UNP Q7Z6Z7
A	-22	SER	-	expression tag	UNP Q7Z6Z7
A	-21	SER	-	expression tag	UNP Q7Z6Z7
A	-20	ILE	-	expression tag	UNP Q7Z6Z7
A	-19	ASP	-	expression tag	UNP Q7Z6Z7
A	-18	LEU	-	expression tag	UNP Q7Z6Z7
A	-17	ILE	-	expression tag	UNP Q7Z6Z7
A	-16	SER	-	expression tag	UNP Q7Z6Z7
A	-15	THR	-	expression tag	UNP Q7Z6Z7
A	-14	SER	-	expression tag	UNP Q7Z6Z7
A	-13	LEU	-	expression tag	UNP Q7Z6Z7
A	-12	TYR	-	expression tag	UNP Q7Z6Z7
A	-11	LYS	-	expression tag	UNP Q7Z6Z7
A	-10	LYS	-	expression tag	UNP Q7Z6Z7
A	-9	ALA	-	expression tag	UNP Q7Z6Z7

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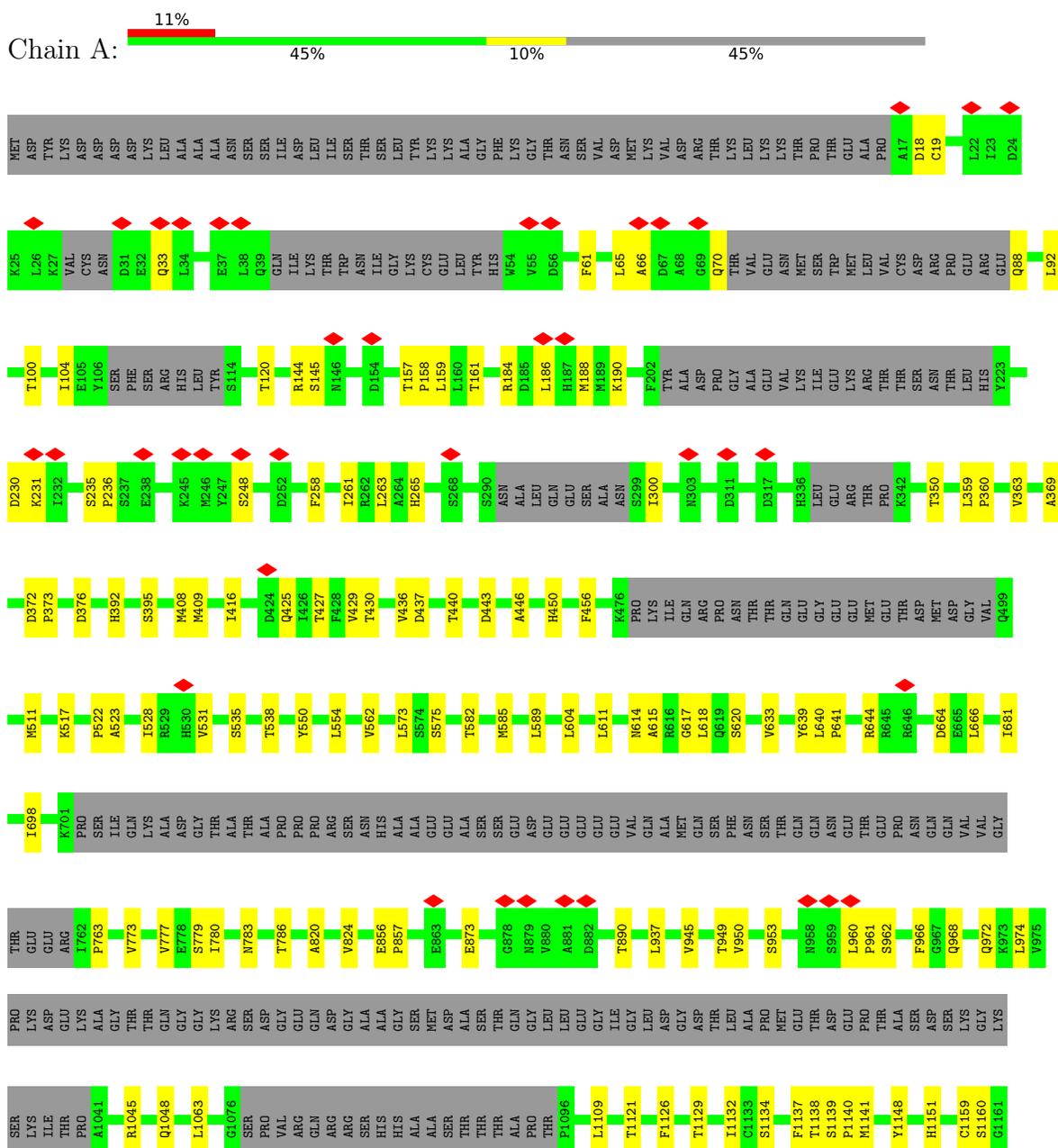
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q7Z6Z7
A	-7	PHE	-	expression tag	UNP Q7Z6Z7
A	-6	LYS	-	expression tag	UNP Q7Z6Z7
A	-5	GLY	-	expression tag	UNP Q7Z6Z7
A	-4	THR	-	expression tag	UNP Q7Z6Z7
A	-3	ASN	-	expression tag	UNP Q7Z6Z7
A	-2	SER	-	expression tag	UNP Q7Z6Z7
A	-1	VAL	-	expression tag	UNP Q7Z6Z7
A	0	ASP	-	expression tag	UNP Q7Z6Z7

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: E3 ubiquitin-protein ligase HUWE1



H4326	T4266	Y4206	M4146	G4086	V4026	T3964	PRO
R4327	F4267	V4207	E4147	D4087	F4027	V3965	PRO
D4328	Y4268	H4208	S4148	R4088	E4028	G3968	VAL
D4329	H4269	L4209	E4149	T4090	D4029	R3971	THR
R4330	K4270	V4210	D4150	Y4091	S4030	G3972	ARG
S4331	Y4271	C4211	Y4151	T4092	Y4031	S3973	GLN
T4332	Q4272	Q4212	F4153	I4093	R4032	T3974	ALA
D4333	S4273	M4213	Y4154	N4094	E4033	T3975	VAL
R4334	M4274	R4214	Q4155	P4095	L4034	H3976	LEU
L4335	S4275	M4215	Q4156	S4096	H4035	H3977	ALA
P4336	I4276	T4216	G4156	S4097	R4036	L3977	HIS
S4337	Q4277	G4217	L4157	H4098	K4037	A3978	ILE
H4338	I4278	A4218	V4158	C4099	S4038	D3979	LYS
R4339	Q4279	R4220	Y4159	N4100	P4039	G3980	ASP
T4340	M4280	K4221	L4160	N4101	E4040	P3981	PRO
C4341	F4281	Q4222	L4161	E4041	E4041	F3982	PRO
F4342	W4282	L4223	E4162	N4102	M4042	A3983	LEU
M4343	R4283	A4224	N4163	H4103	K4043	V3984	LEU
Q4344	A4284	A4225	D4164	L4104	M4044	L3985	LYS
L4345	L4285	F4226	V4165	S4105	R4045	D3986	VAL
D4346	R4286	L4227	S4166	Y4106	L4046	V3987	ALA
L4347	S4287	E4228	T4167	K4107	L4046	D3988	LEU
F4348	F4288	G4229	L4168	K4108	Y4047	Y3988	THR
A4349	D4289	F4230	C4169	F4109	I4048	I3989	ALA
Y4350	Q4290	Y4231	Y4170	V4110	V4049	R3990	THR
E4351	A4291	E4232	D4171	G4111	F4050	V3991	PRO
S4352	D4292	I4233	L4172	R4112	E4051	D3993	LEU
F4353	R4293	I4234	T4173	I4113	G4052	F3994	LEU
A4354	A4294	P4235	F4174	V4114	E4053	D3995	ASP
K4355	K4295	K4236	S4175	A4115	E4054	V3996	PHE
L4356	F4296	R4237	T4176	K4116	G4055	K3997	PHE
R4357	L4297	L4238	E4177	A4117	Q4056	R3998	SER
H4358	Q4298	I4239	V4178	V4118	D4057	K3999	ARG
M4359	F4299	S4240	Q4179	Y4119	A4058	Y4000	GLU
L4360	Y4300	I4241	E4180	D4120	G4059	F4001	PRO
L4361	T4301	F4242	F4181	M4121	G4060	R4002	SER
L4362	C4302	T4243	G4182	R4122	L4061	Q4003	SER
A4363	T4303	E4244	V4183	L4123	L4062	E4004	MET
I4364	S4304	Q4245	C4184	E4125	R4063	L4005	HIS
GLN	K4305	E4246	E4185	C4126	E4064	E4006	ALA
GLU	K4306	L4247	E4186	Y4127	V4065	R4007	LYS
CYS	P4307	E4248	V4187	Y4128	Y4066	D4009	ALA
SER	L4308	L4249	R4187	F4129	M4067	E4010	GLN
GLU	L4309	L4250	D4188	T4129	I4068	G4011	THR
GLY	Q4309	I4251	L4189	R4130	I4069	L4012	ASP
GLY	G4310	S4252	K4190	S4131	S4070	R4013	GLY
LEU	F4311	G4253	PRO	F4132	R4071	K4014	ASP
ALA	A4312	L4254	ASN	Y4133	E4072	E3960	VAL
	A4313	P4255	GLY	K4134	M4073	R3963	ARG
	L4314	T4256	ALA	H4135	F4074		GLU
	E4315	I4257	ASN	I4136	M4075		LYS
	M4316	I4257	ILE	I4137	P4076		
	G4317	D4258	LEU	C4138	M4077		
	M4318	I4259	V4198	K4139	M4077		
	C4319	D4260	T4199	S4140	Y4078		
	I4320	D4261	T4199	A4079	A4079		
	K4321	L4262	E4200	L4080	F4081		
	K4322	K4263	E4201	F4081	R4023		
	F4323	S4264	K4203	Y4143	D4024		
	Q4324	M4265	K4204	T4144	H4025		
	I4325		E4205	D4145			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	762898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; standard correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.68	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (\AA)	300.3, 300.3, 300.3	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	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	0.36	0/19509	0.56	0/26411

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	19165	19554	19539	262	0
All	All	19165	19554	19539	262	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 7.

The worst 5 of 262 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:4056:GLN:OE1	1:A:4057:ASP:N	2.10	0.84
1:A:1109:LEU:HD22	1:A:1138:THR:HG22	1.63	0.80
1:A:2227:ARG:NH2	1:A:3184:GLU:OE1	2.16	0.79
1:A:1829:GLU:OE2	1:A:2082:TYR:OH	2.01	0.77
1:A:1134:SER:O	1:A:1138:THR:HG23	1.83	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2369/4411 (54%)	2308 (97%)	61 (3%)	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	2149/3839 (56%)	2117 (98%)	32 (2%)	65 85

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4203	LYS
1	A	4228	GLU
1	A	2185	THR
1	A	2144	SER
1	A	4273	SER

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	1258	ASN

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Mol	Chain	Res	Type
1	A	3302	GLN
1	A	4343	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 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](#)

There are no chain breaks in this entry.

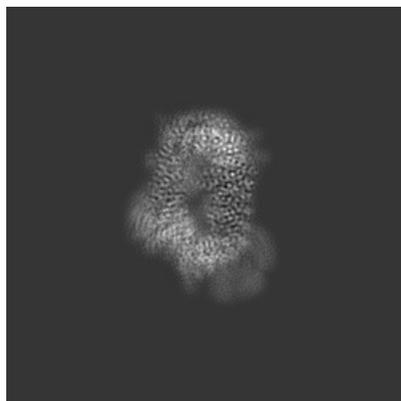
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22427. These allow visual inspection of the internal detail of the map and identification of artifacts.

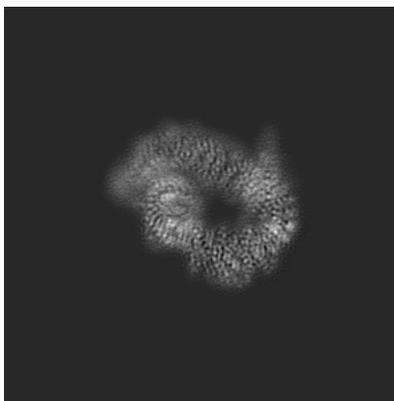
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

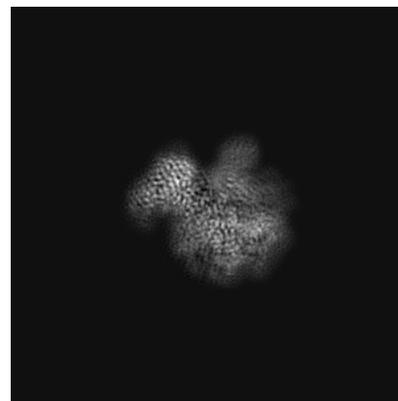
6.1.1 Primary map



X

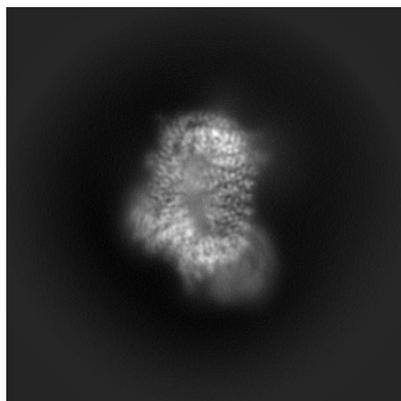


Y

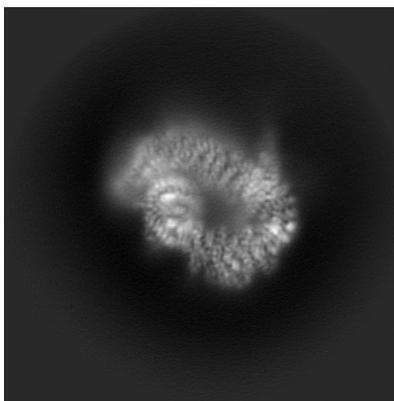


Z

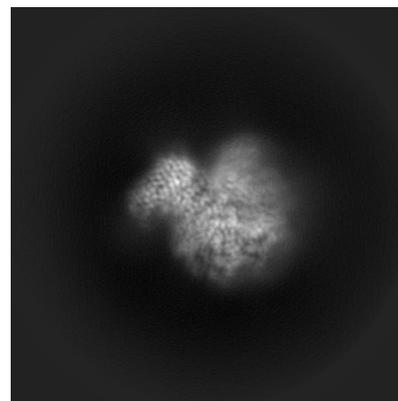
6.1.2 Raw map



X



Y

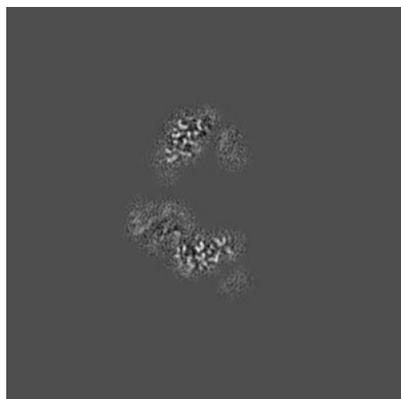


Z

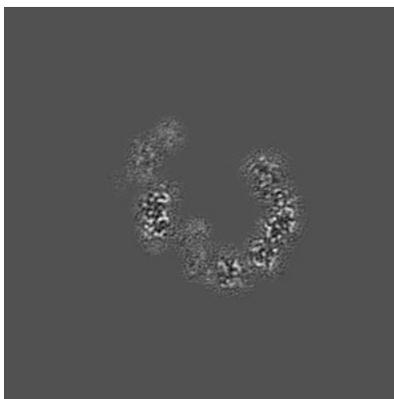
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

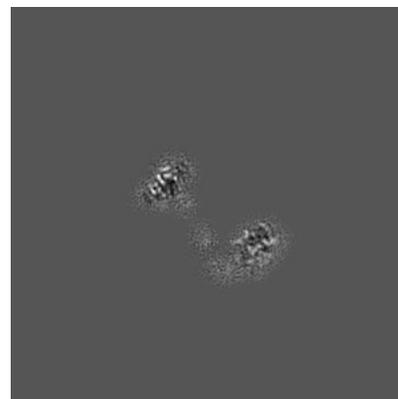
6.2.1 Primary map



X Index: 182

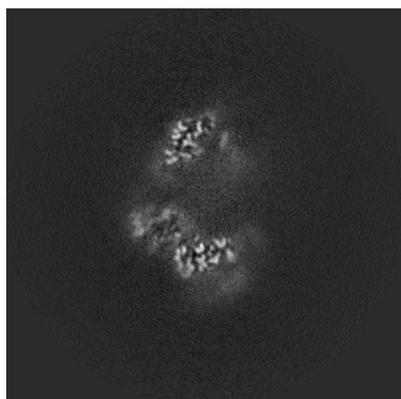


Y Index: 182

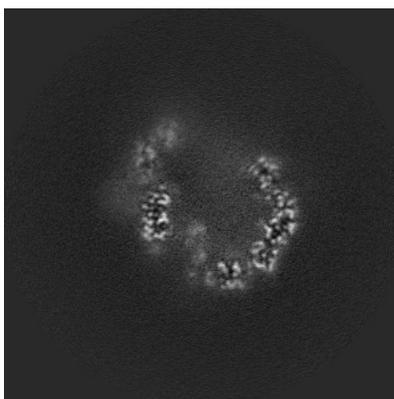


Z Index: 182

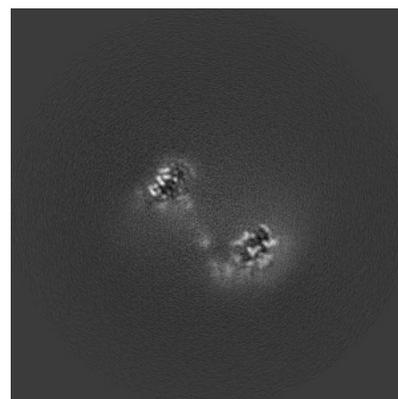
6.2.2 Raw map



X Index: 182



Y Index: 182

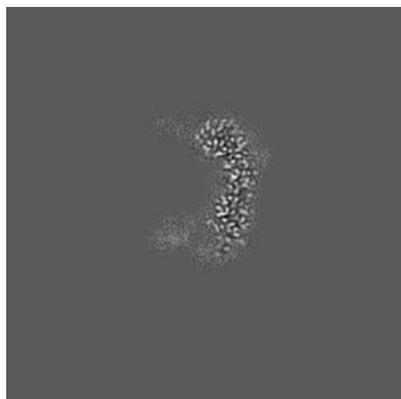


Z Index: 182

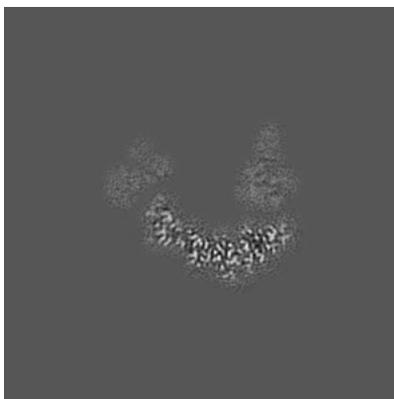
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

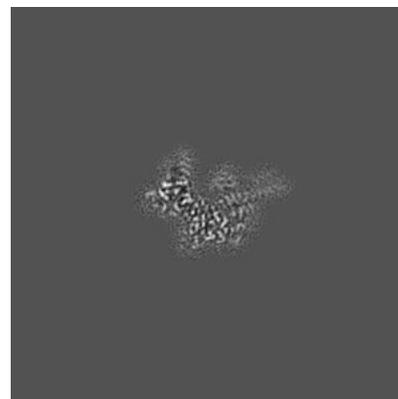
6.3.1 Primary map



X Index: 149

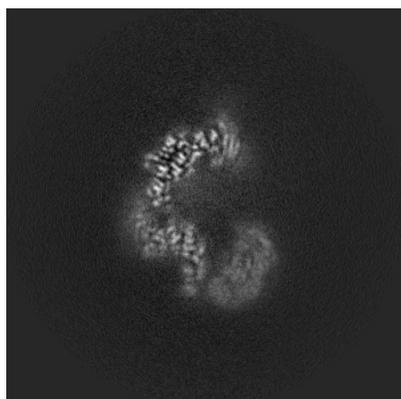


Y Index: 202

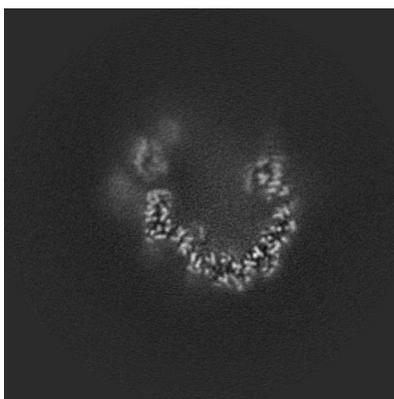


Z Index: 246

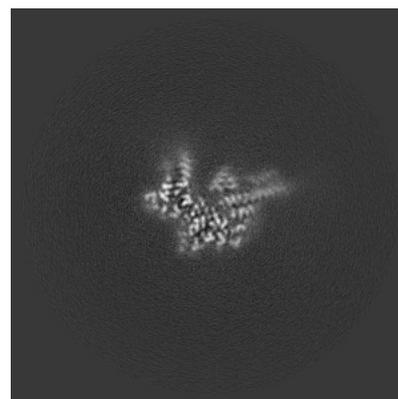
6.3.2 Raw map



X Index: 203



Y Index: 189

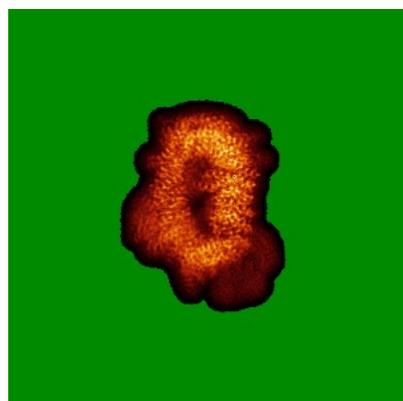


Z Index: 246

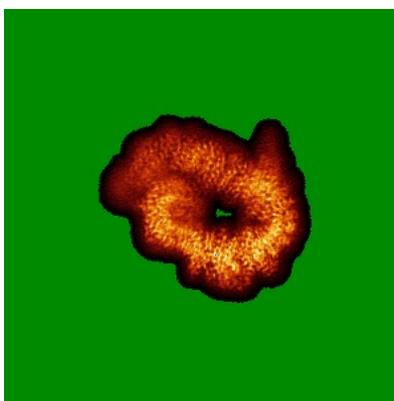
The images above show the largest variance slices of the map in three orthogonal directions.

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

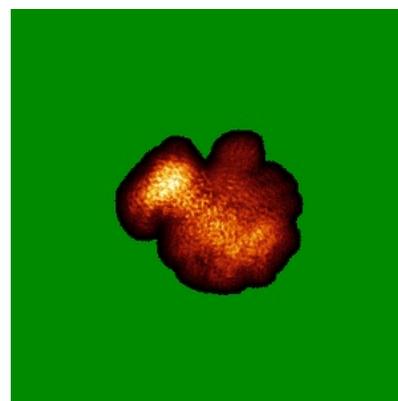
6.4.1 Primary map



X

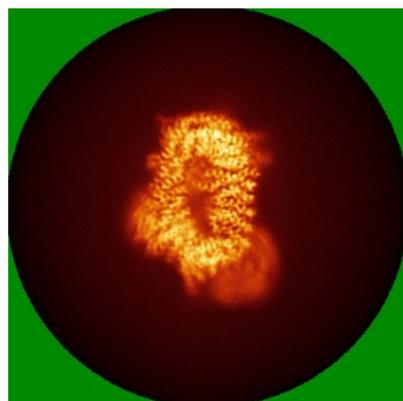


Y

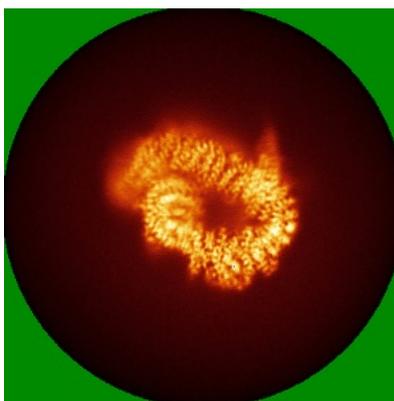


Z

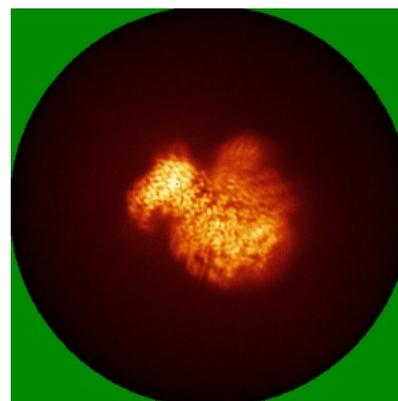
6.4.2 Raw map



X



Y

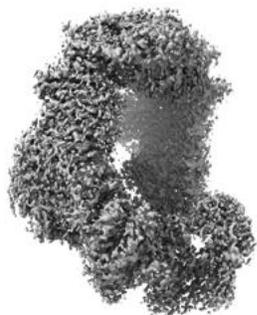


Z

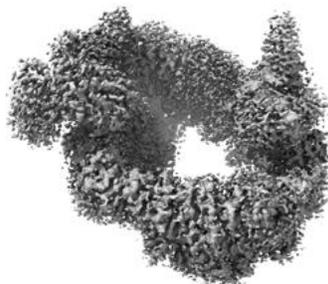
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

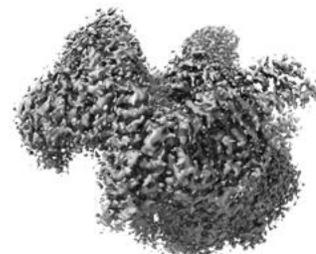
6.5.1 Primary map



X



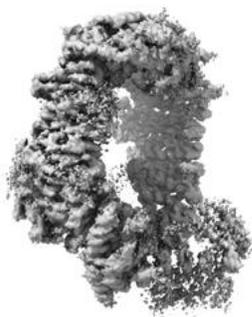
Y



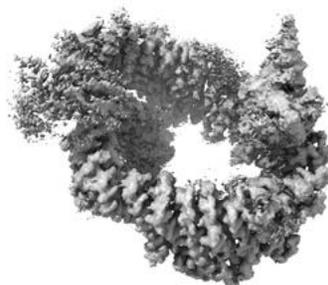
Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

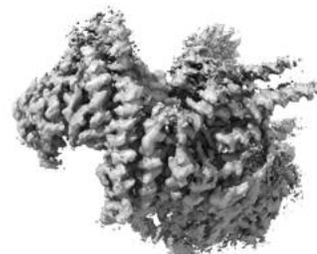
6.5.2 Raw map



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.

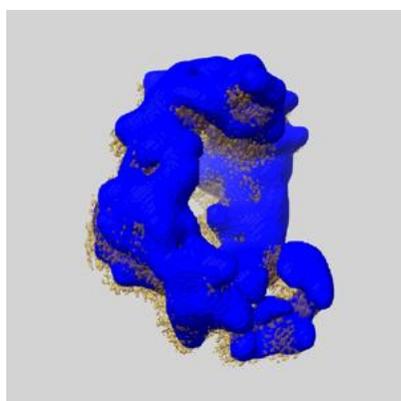
6.6 Mask visualisation [i](#)

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

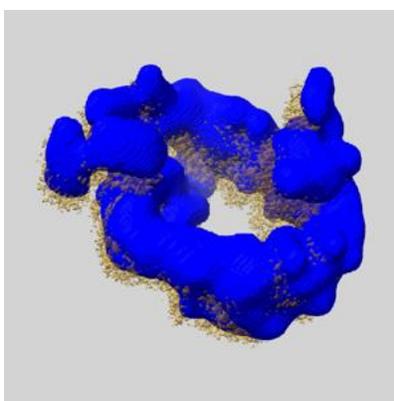
A mask typically either:

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

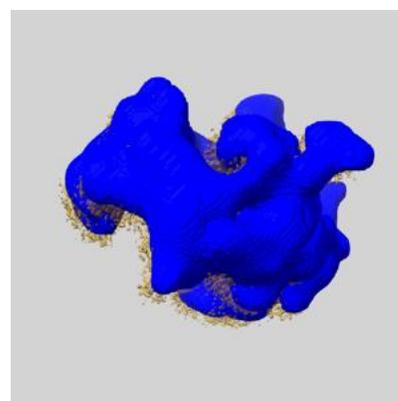
6.6.1 emd_22427_msk_1.map [i](#)



X



Y

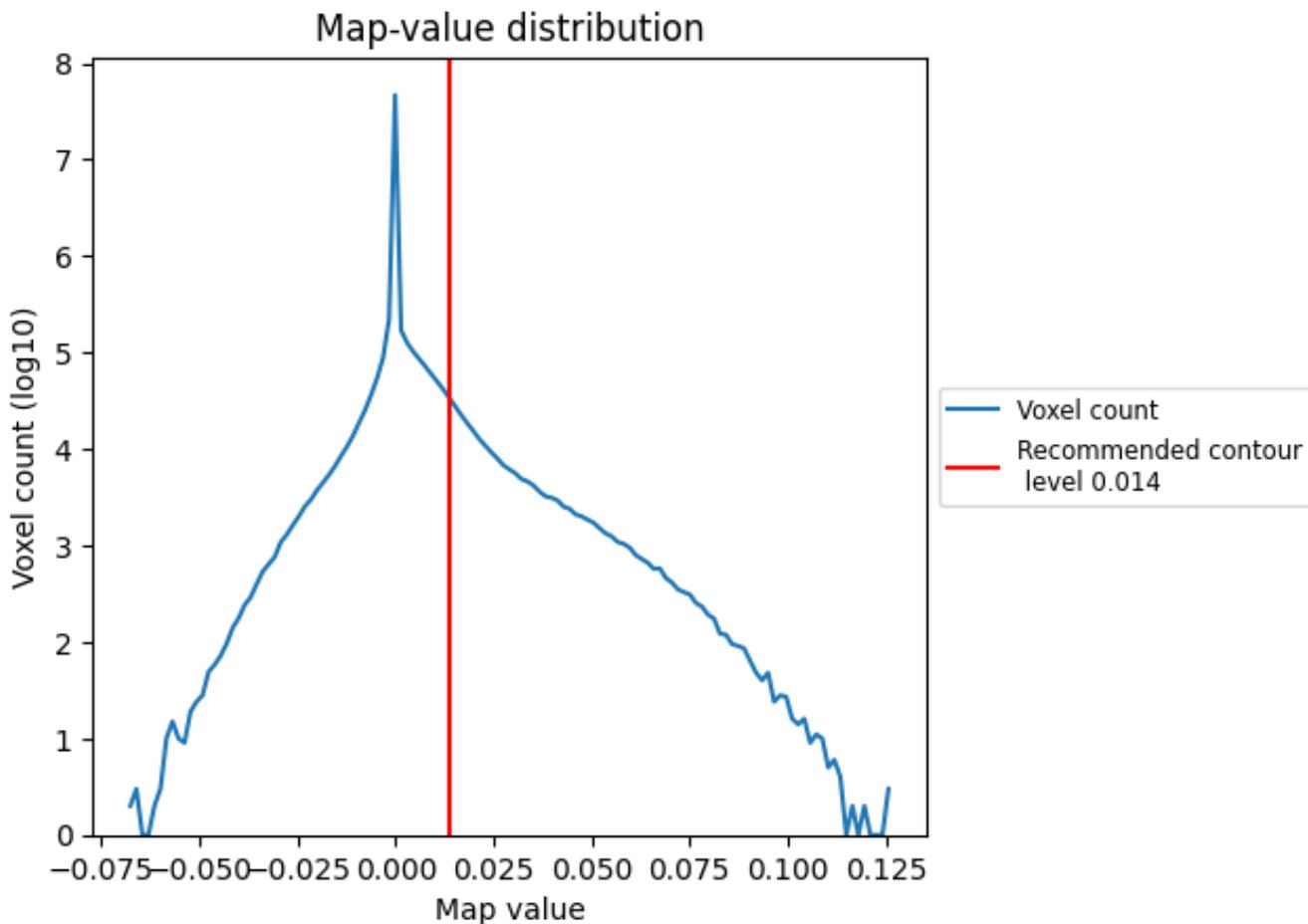


Z

7 Map analysis [i](#)

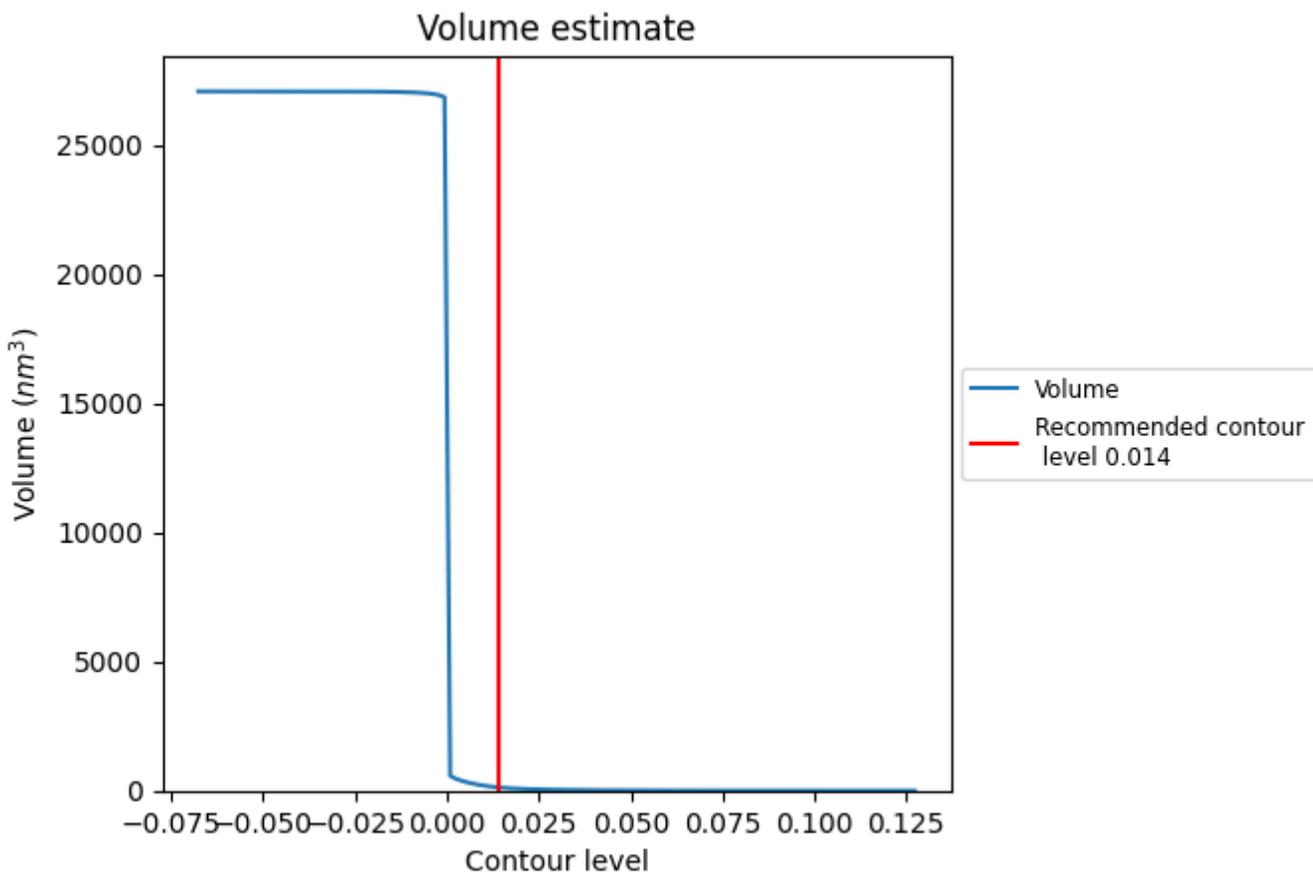
This section contains the results of statistical analysis of the map.

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.

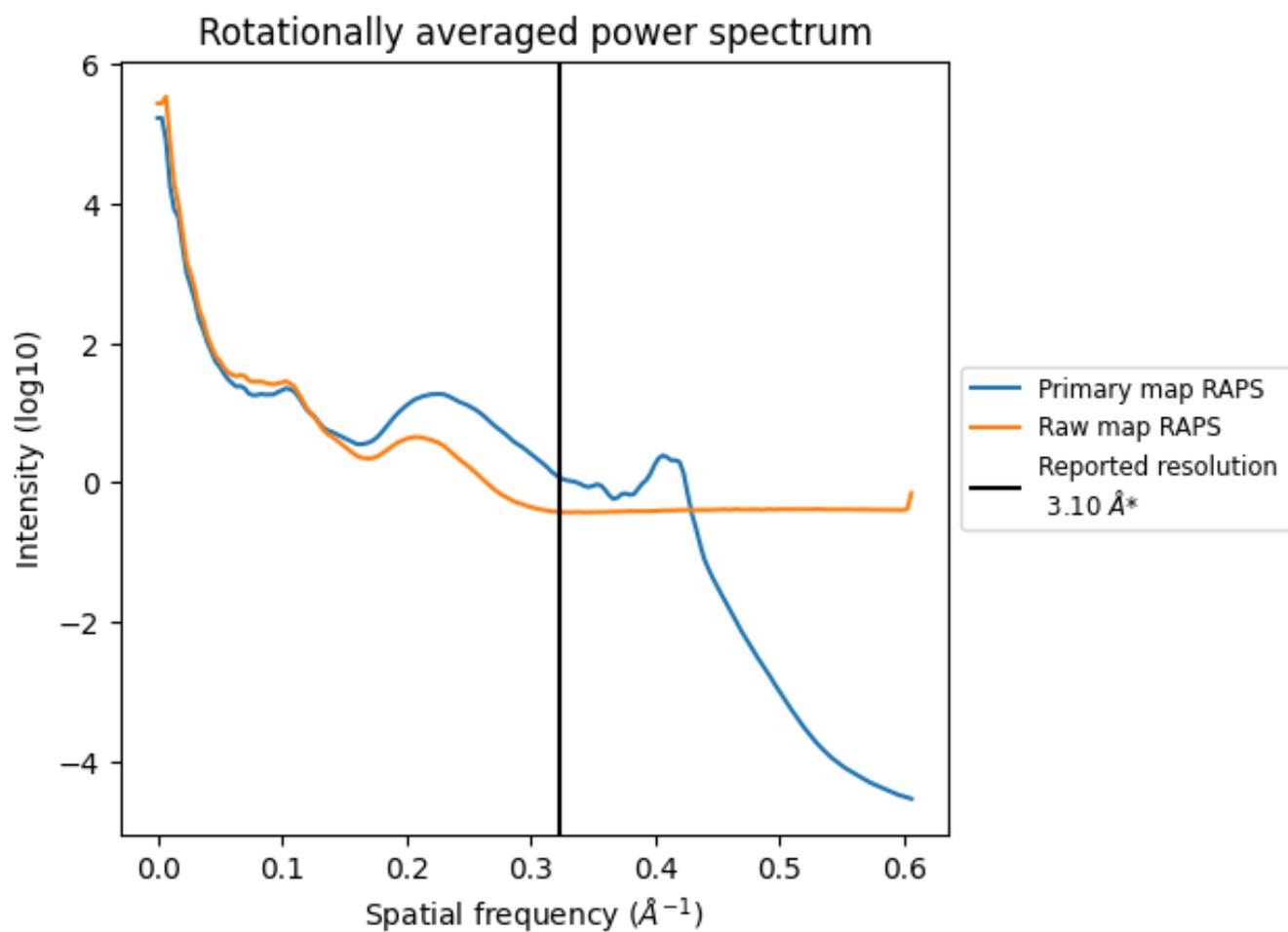
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 126 nm^3 ; this corresponds to an approximate mass of 114 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](#)

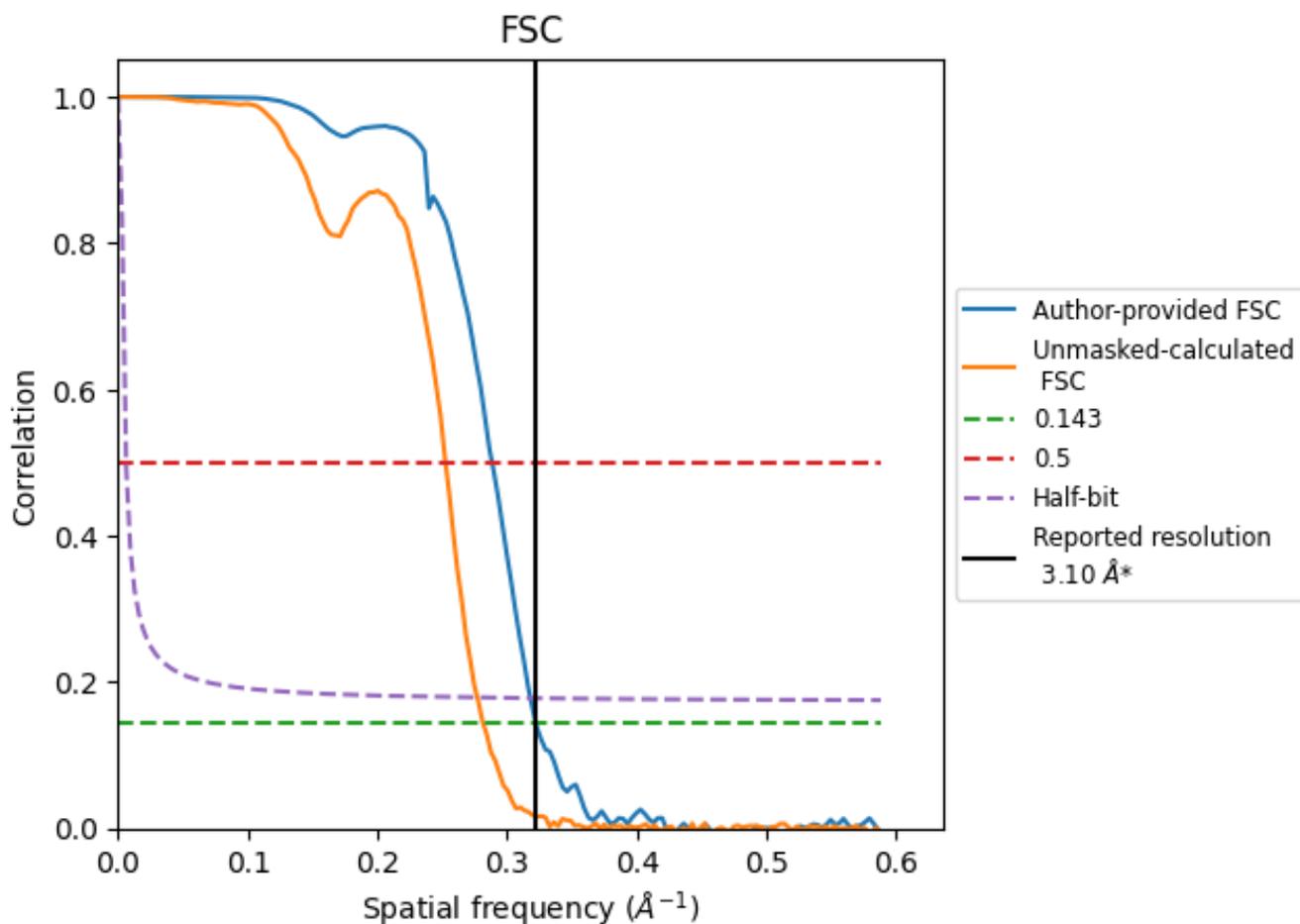


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

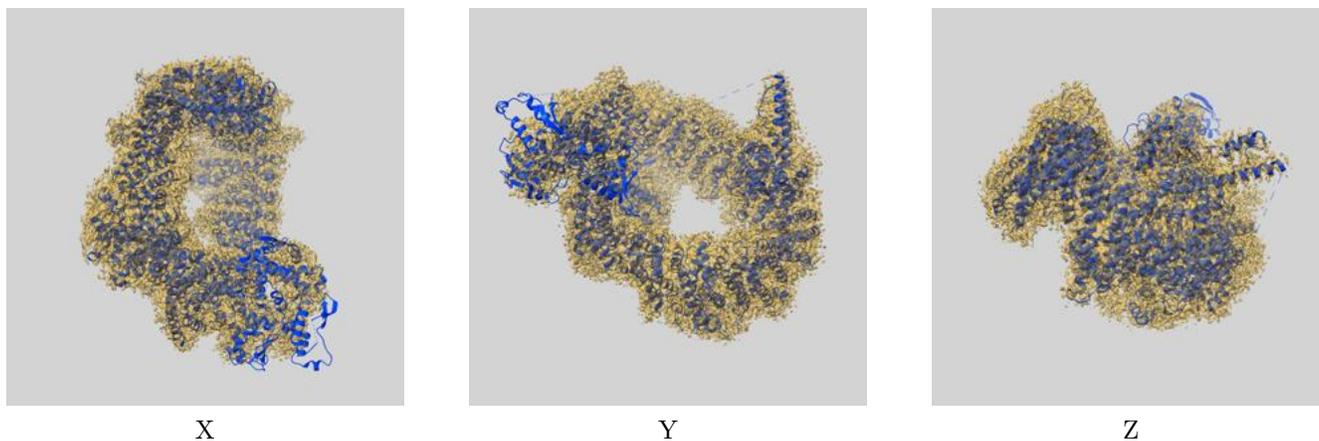
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.47	3.14
Unmasked-calculated*	3.55	3.96	3.61

*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 3.55 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

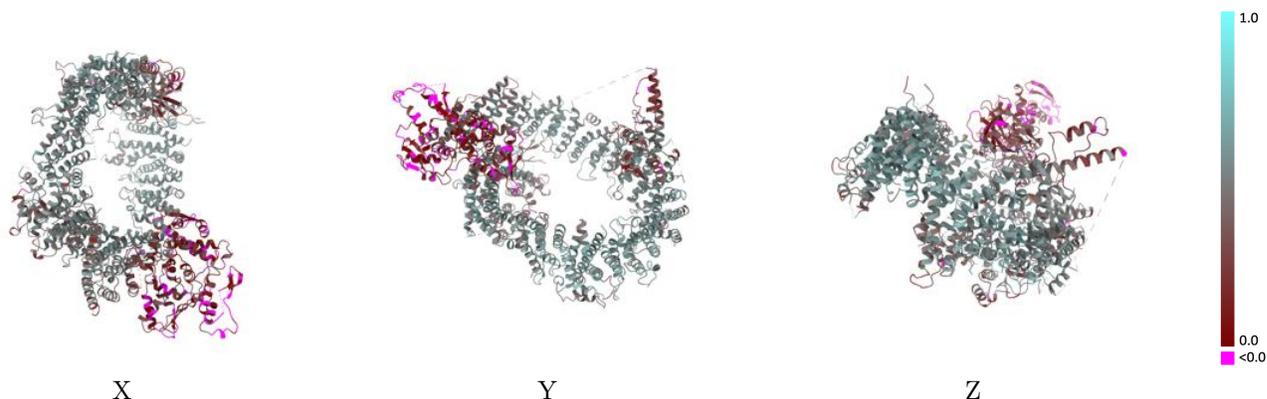
This section contains information regarding the fit between EMDB map EMD-22427 and PDB model 7JQ9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



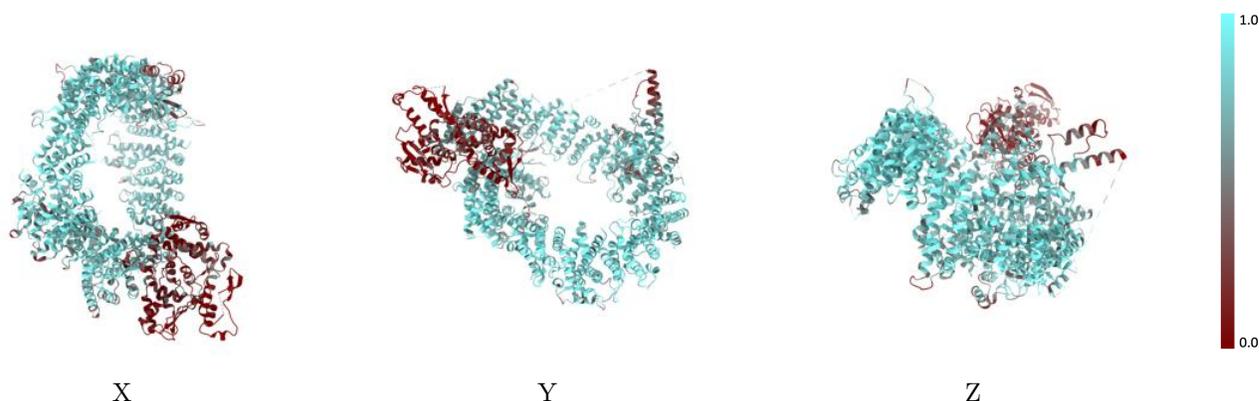
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



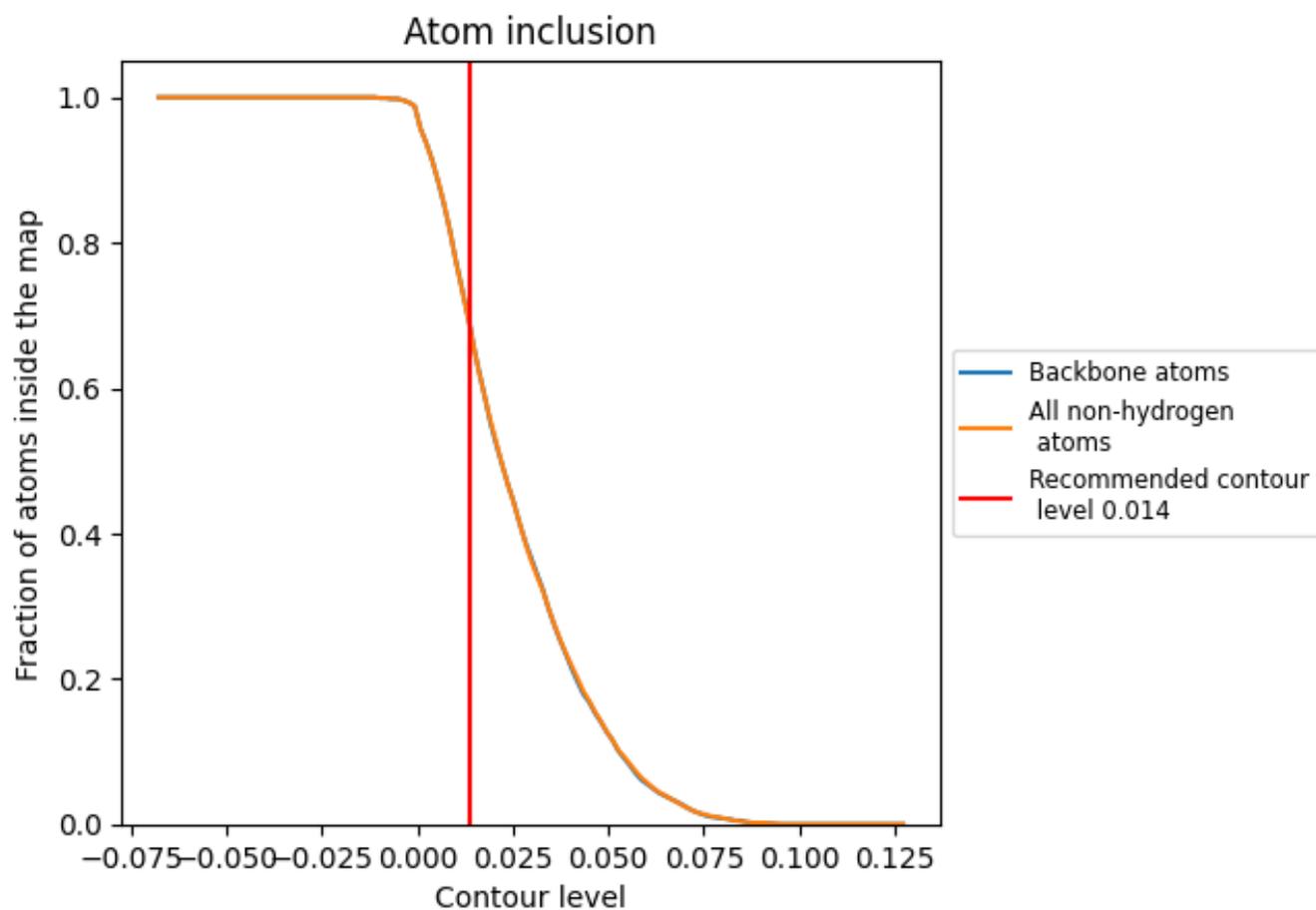
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6800	 0.4290
A	 0.6810	 0.4290

