



wwPDB EM Validation Summary Report ⓘ

Jan 13, 2025 – 01:47 PM JST

PDB ID : 8XXT
EMDB ID : EMD-38760
Title : ASFV RNAP M1249L C-tail occupied complex2 (MCOC2)
Authors : Zhu, G.L.; Zhu, Y.; Zhu, Z.X.; Sun, F.; Zheng, H.X.
Deposited on : 2024-01-19
Resolution : 2.85 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.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) : 2.40

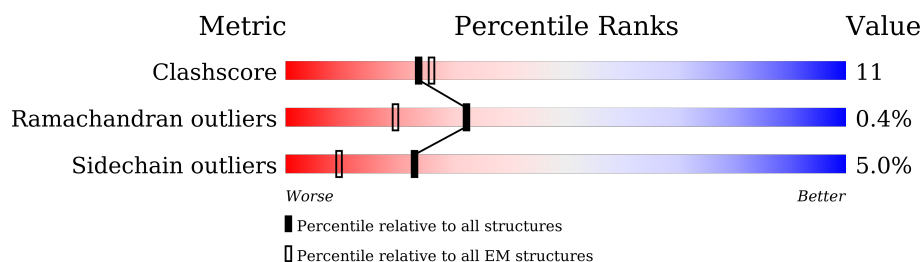
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 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	1441	
2	B	1235	
3	C	358	
4	D	205	
5	E	139	
6	F	334	
7	G	105	
8	H	80	

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Mol	Chain	Length	Quality of chain
9	I	1170	<div><div><div></div><div></div><div></div><div></div></div><div>23%39%14%45%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 35783 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-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1415	Total	C	N	O	S	0	0
			11244	7135	1955	2092	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1226	Total	C	N	O	S	0	0
			9701	6124	1706	1819	52		

- Molecule 3 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	358	Total	C	N	O	S	0	0
			2907	1885	481	529	12		

- Molecule 4 is a protein called DNA-directed RNA polymerase RPB5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	205	Total	C	N	O	S	0	0
			1669	1088	278	295	8		

- Molecule 5 is a protein called C147L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	129	Total	C	N	O	S	0	0
			1021	648	167	200	6		

- Molecule 6 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	334	Total	C	N	O	S	0	0
			2687	1726	444	503	14		

- Molecule 7 is a protein called C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	105	Total	C	N	O	S	0	0
			816	507	141	153	15		

- Molecule 8 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	69	Total	C	N	O	S	0	0
			553	362	89	95	7		

- Molecule 9 is a protein called M1249L.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	638	Total	C	N	O	S	0	0
			5177	3329	858	968	22		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	3	Total	Zn	0
			3	3	
10	B	1	Total	Zn	0
			1	1	
10	G	2	Total	Zn	0
			2	2	
10	H	1	Total	Zn	0
			1	1	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

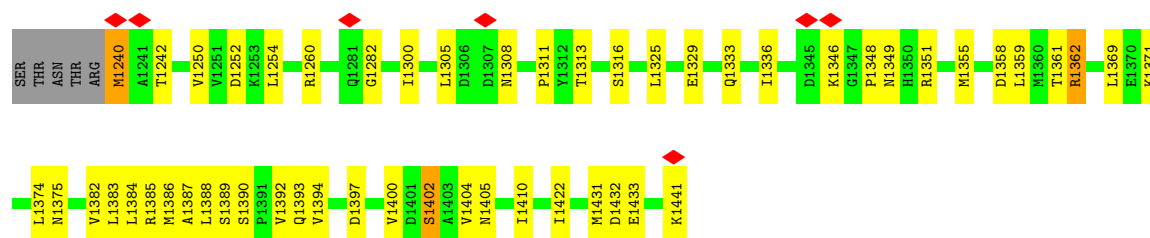
Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

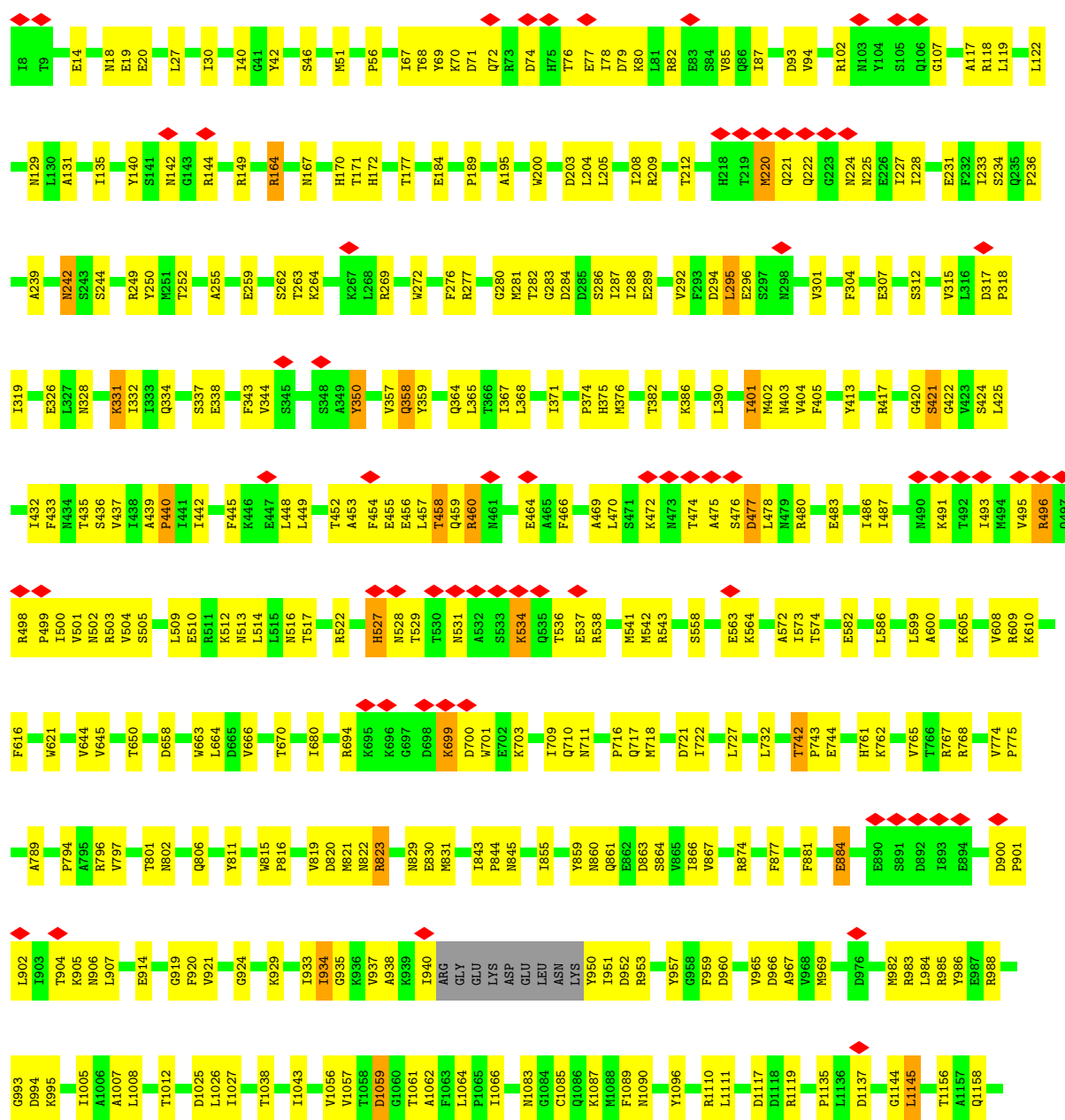
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase subunit

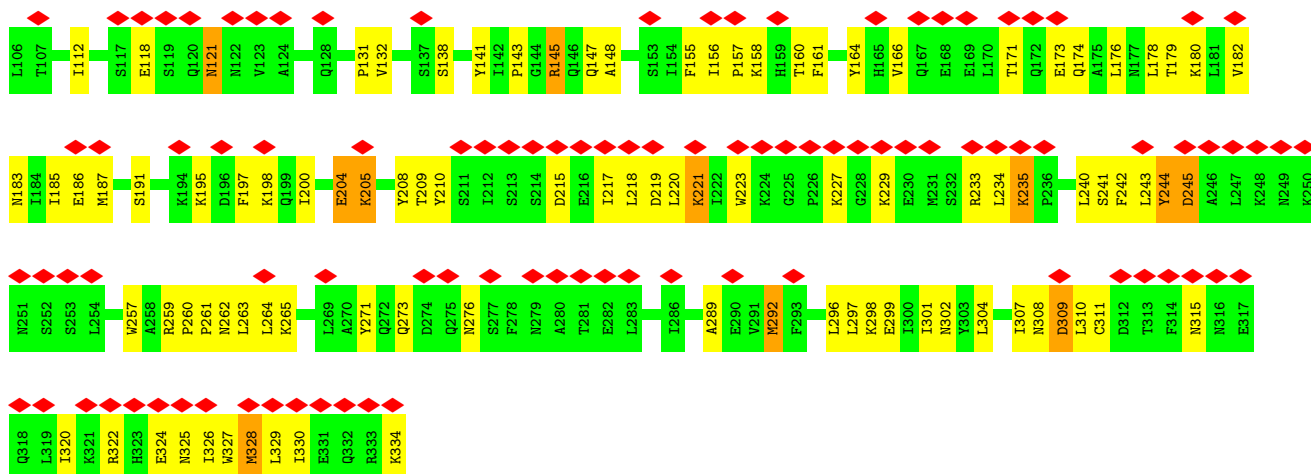




• Molecule 2: DNA-directed RNA polymerase subunit beta



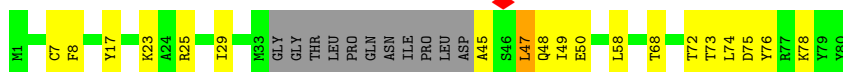




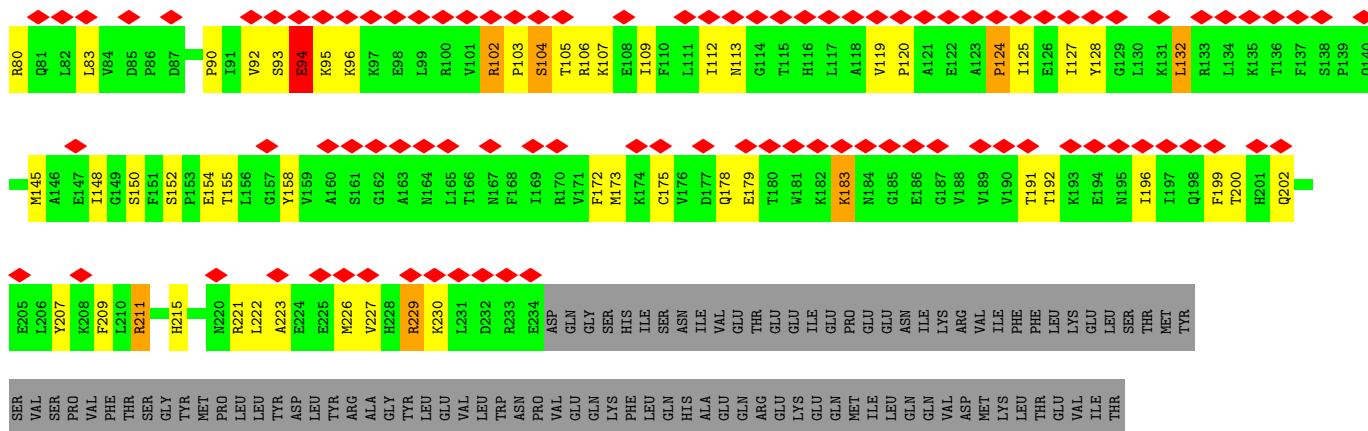
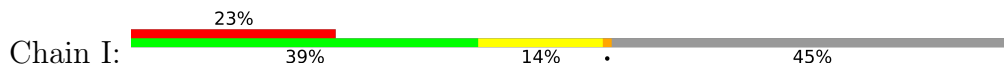
• Molecule 7: C122R



• Molecule 8: DNA-directed RNA polymerase RPB10 homolog



• Molecule 9: M1249L



V1162	V1165	R1166	E1172	T1177	K1181	L1182	P1186	M1192	I1193	F1194	G1195	E1196	D1197	F1198	V1199	C1200	M1207	D1208	D1209	I1210	S1214	S1215	P1216	F1219	E1221	D1222	I1223	I1224	D1225	R1226	L1227	D1228	S1232	I1233	E1234	D1235	V1236	S1239	L1240	D1241	V1242	P1248	Q1249													
L1027	D1028	I1029	V1033	I1034	I1037	E1050	S1060	M1061	D1070	R1074	I1075	F1076	L1077	Y1078	N1079	N1090	K1091	I1094	H1095	V1096	E1097	R1098	L1099	V1100	K1101	H1102	L1103	S1104	Y1105	E1106	E1107	K1108	E1109	E1112	K1113	I1142	F1149	L1150	T1151	L1152	Y1153	E1154	I1155	P1158	S1159	W1160	V1161									
I960	Y961	D962	H963	L964	S965	Q966	P967	E968	L969	V970	H971	D972	Y973	Y974	N975	N976	Y977	K978	D979	Q980	Y981	D982	K983	E984	K985	M986	S987	I1103	I1223	E1106	E1107	K1108	E1109	E1112	K1113	I1142	F1149	L1150	T1151	L1152	Y1153	E1154	I1155	P1158	S1159	W1160	V1161									
R897	C898	S899	Y903	L904	Q905	H906	E907	Q910	L911	N912	I913	K914	K915	V916	Q917	T918	A919	L920	K921	A922	S923	L924	E925	F926	N927	T928	Y930	A931	F932	Y933	E934	S935	R936	C937	P938	K939	G940	G941	L942	H943	D944	F945	Q946	D947	K948	K949	C950	V951	K952	C953	G954	L955	F956	T957	Y958	I959
E811	Q812	A817	Q818	Q819	Q820	F821	Y822	D826	A832	D833	Q834	R835	T836	E840	Y841	K842	S847	D851	E852	R853	G854	L855	Y864	K865	A866	V867	D868	S869	S870	K871	K872	P873	A874	E875	I876	T879	R880	K881	D882	V883	I884	K885	D888	N889	H890	Y891	A892	D895	L896							
ARG	LEU	ASN	ASP	ILE	TYR	PHE	GLN	GLU	SER	LEU	ARG	VAL	TRP	GLY	GLY	ARG	ASP	GLU	GLU	K772	T773	S774	T775	I776	I777	R780	A781	Y782	E783	L784	F785	L786	K787	Y788	L789	Q790	N791	A792	P793	N794	N796	F795	S797	E798	L799	A800	E801	F802	K803	T804	Y805	E806	N807	A808	Y809	G810
A890	A891	T892	V893	A894	R895	I896	D897	G898	S899	I700	P701	M702	H703	K704	TRR	TRR	PRO	LYS	ALA	GLU	ALA	TRR	GLU	PHE	LYS	LYS	ILE	ILE	HIS	GLN	ASN	ARG	GLY	GLY	ASP	ASP	LYS	ILE	TRR	TRR	TRR	SER	LYS	TRR	ARG	PRO	PRO	ASP	P885	M886	Y887	D888	Y889			
GLN	ALA	ARG	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ALA	ILE	GLY	GLY	ASP	TRP	TRP	ASN	ASN	GLU	ALA	TRP	TRP	GLU	GLU	VAL	ILE	HIS	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU			
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU			
GLN	ALA	ARG	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU			
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
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LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL	VAL	VAL	VAL	PRO	GLU	VAL	THR	THR	ALA	ALA	GLY	THR	GLN	LEU	LEU				
LYS	LYS	GLN	TRP	GLU	ASP	VAL	PHE	GLN	LYS	ILE	GLY	GLY	ASP	PRO	LEU	GLN	ASN	ALA	ALA	TRR	TRP	TRP	GLU	GLU	THR	LYS	LEU	GLN	ASP	ASP	THR	LYS	VAL	ASN	ASN	VAL	VAL																			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83920	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	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.226	Depositor
Minimum map value	-1.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0/11462	0.50	1/15525 (0.0%)
2	B	0.30	0/9896	0.51	1/13394 (0.0%)
3	C	0.30	0/2969	0.48	0/4012
4	D	0.28	0/1708	0.51	0/2311
5	E	0.28	0/1033	0.49	0/1398
6	F	0.29	0/2740	0.52	0/3709
7	G	0.31	0/828	0.56	1/1109 (0.1%)
8	H	0.32	0/563	0.61	2/758 (0.3%)
9	I	0.27	0/5298	0.51	2/7172 (0.0%)
All	All	0.29	0/36497	0.51	7/49388 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	124	PRO	CA-N-CD	-8.92	99.01	111.50
1	A	1204	PRO	CA-N-CD	-8.27	99.92	111.50
8	H	47	LEU	CA-CB-CG	6.48	130.20	115.30
2	B	440	PRO	CA-N-CD	-5.58	103.68	111.50
8	H	47	LEU	CB-CG-CD1	5.37	120.13	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	11244	0	11362	214	0
2	B	9701	0	9657	285	0
3	C	2907	0	2982	52	0
4	D	1669	0	1713	42	0
5	E	1021	0	1054	25	0
6	F	2687	0	2721	84	0
7	G	816	0	814	21	0
8	H	553	0	580	27	0
9	I	5177	0	5136	130	0
10	A	3	0	0	0	0
10	B	1	0	0	0	0
10	G	2	0	0	0	0
10	H	1	0	0	0	0
11	A	1	0	0	0	0
All	All	35783	0	36019	770	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 770 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)
8:H:48:GLN:HB2	9:I:821:PHE:H	1.24	1.03
3:C:29:LEU:HD22	8:H:23:LYS:HD3	1.54	0.88
4:D:192:MET:O	4:D:193:HIS:ND1	2.08	0.86
2:B:491:LYS:HE2	2:B:527:HIS:HB3	1.60	0.84
2:B:1161:MET:O	2:B:1163:THR:N	2.13	0.81

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	1407/1441 (98%)	1351 (96%)	51 (4%)	5 (0%)	30	49
2	B	1222/1235 (99%)	1130 (92%)	86 (7%)	6 (0%)	25	43
3	C	356/358 (99%)	338 (95%)	18 (5%)	0	100	100
4	D	203/205 (99%)	196 (97%)	7 (3%)	0	100	100
5	E	125/139 (90%)	108 (86%)	17 (14%)	0	100	100
6	F	332/334 (99%)	298 (90%)	30 (9%)	4 (1%)	11	23
7	G	103/105 (98%)	95 (92%)	7 (7%)	1 (1%)	13	26
8	H	65/80 (81%)	59 (91%)	6 (9%)	0	100	100
9	I	630/1170 (54%)	588 (93%)	40 (6%)	2 (0%)	37	55
All	All	4443/5067 (88%)	4163 (94%)	262 (6%)	18 (0%)	32	49

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	582	MET
2	B	421	SER
2	B	1162	GLN
2	B	1202	ASP
9	I	94	GLU

5.3.2 Protein sidechains ⓘ

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	1250/1270 (98%)	1200 (96%)	50 (4%)	27	51
2	B	1066/1074 (99%)	1022 (96%)	44 (4%)	26	50
3	C	327/327 (100%)	312 (95%)	15 (5%)	23	44
4	D	185/185 (100%)	173 (94%)	12 (6%)	14	29
5	E	119/129 (92%)	113 (95%)	6 (5%)	20	40
6	F	308/308 (100%)	283 (92%)	25 (8%)	9	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	96/96 (100%)	90 (94%)	6 (6%)	15	30
8	H	61/70 (87%)	59 (97%)	2 (3%)	33	59
9	I	572/1057 (54%)	534 (93%)	38 (7%)	14	28
All	All	3984/4516 (88%)	3786 (95%)	198 (5%)	23	40

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	101	ASN
6	F	235	LYS
4	D	177	ARG
6	F	85	ASP
6	F	328	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	147	GLN
8	H	69	HIS
8	H	48	GLN
9	I	819	GLN
1	A	1078	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

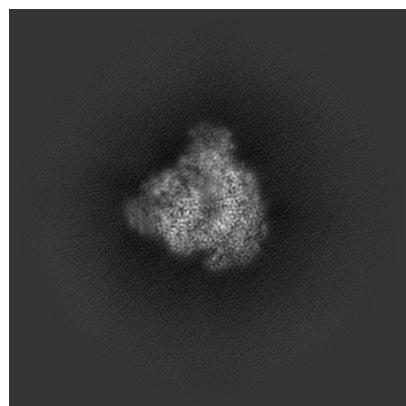
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38760. These allow visual inspection of the internal detail of the map and identification of artifacts.

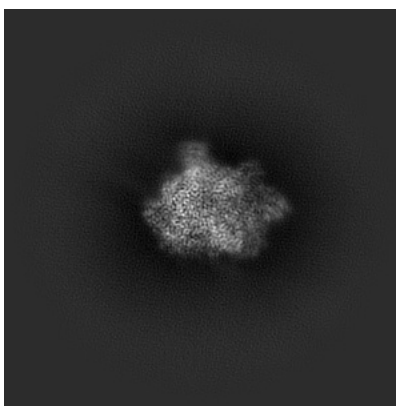
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

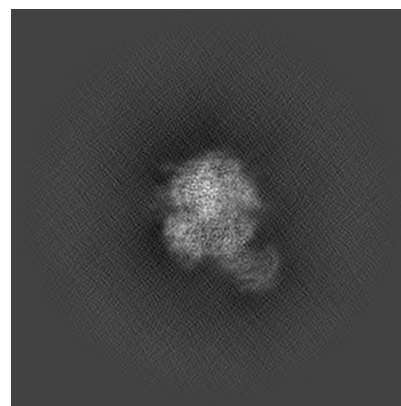
6.1.1 Primary map



X

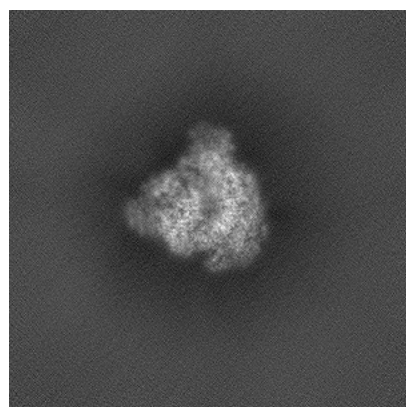


Y

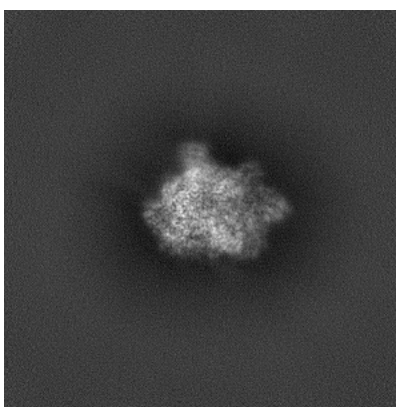


Z

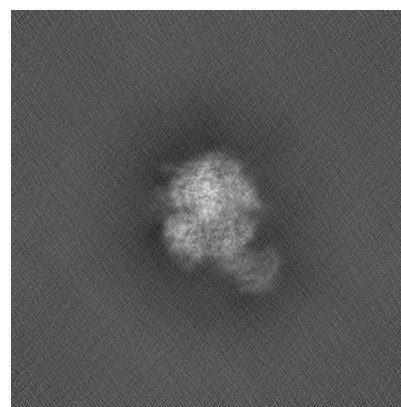
6.1.2 Raw map



X



Y

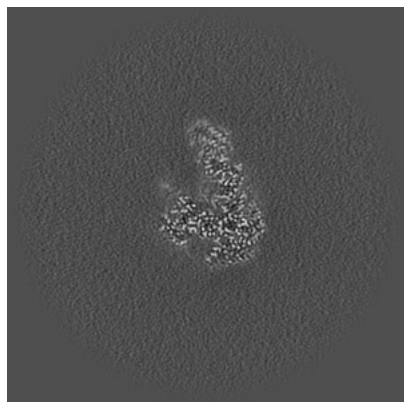


Z

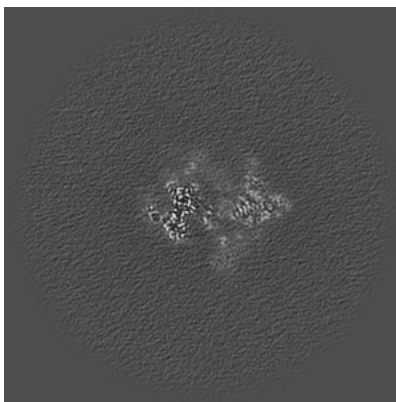
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

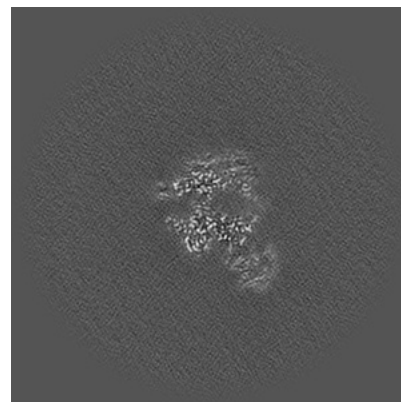
6.2.1 Primary map



X Index: 256

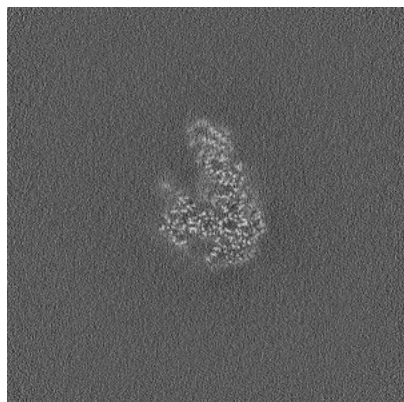


Y Index: 256

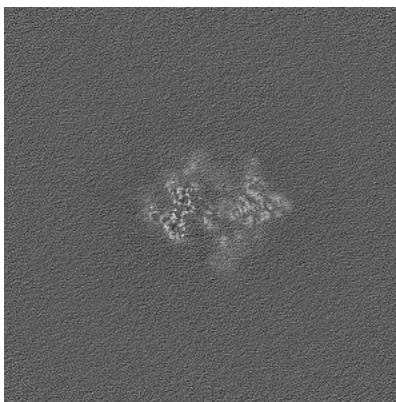


Z Index: 256

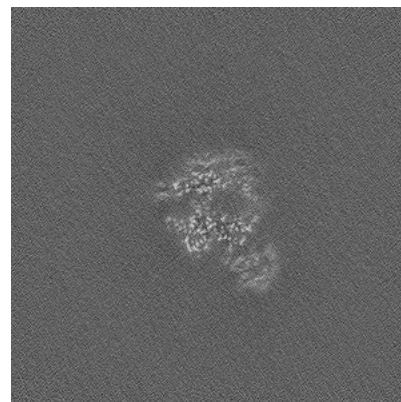
6.2.2 Raw map



X Index: 256



Y Index: 256

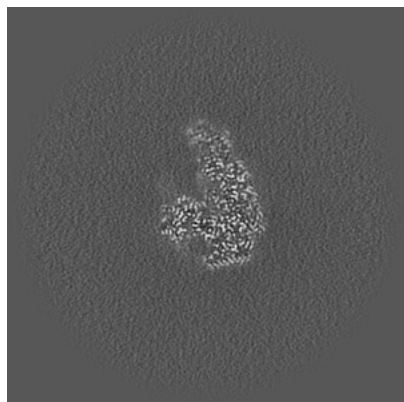


Z Index: 256

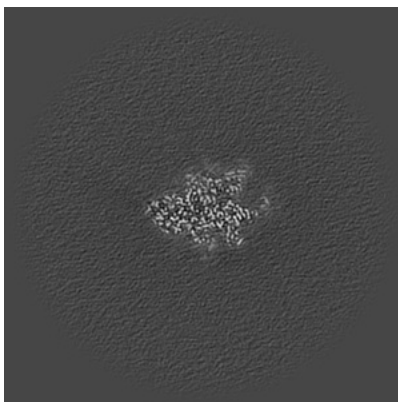
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

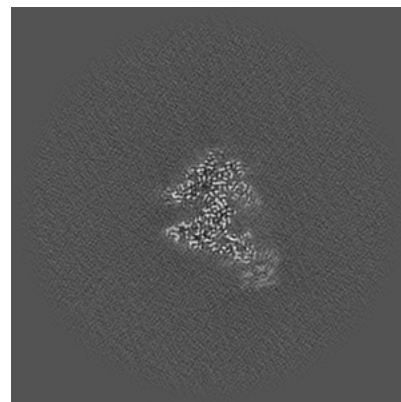
6.3.1 Primary map



X Index: 252

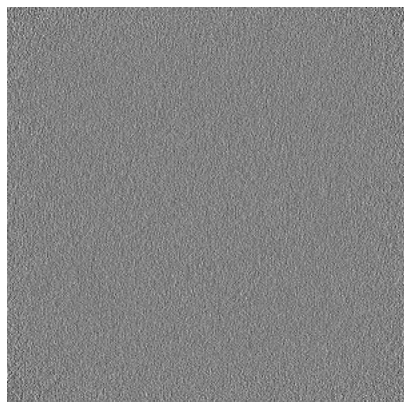


Y Index: 287

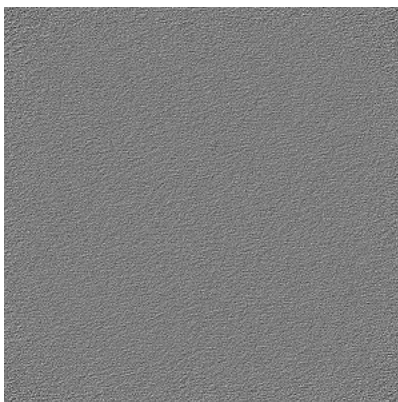


Z Index: 236

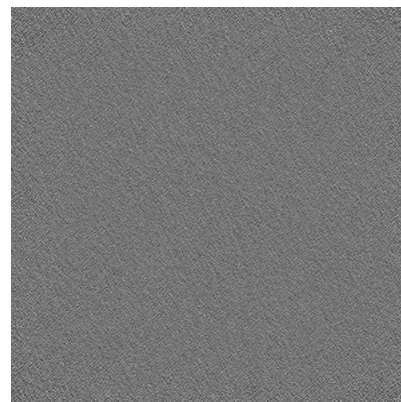
6.3.2 Raw map



X Index: 0



Y Index: 0

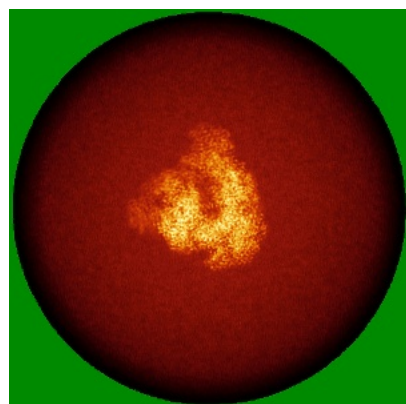


Z Index: 0

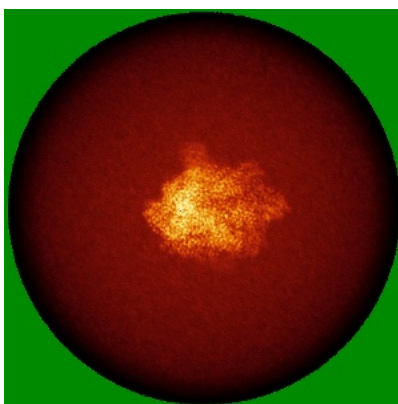
The images above show the largest variance slices of the map in three orthogonal directions.

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

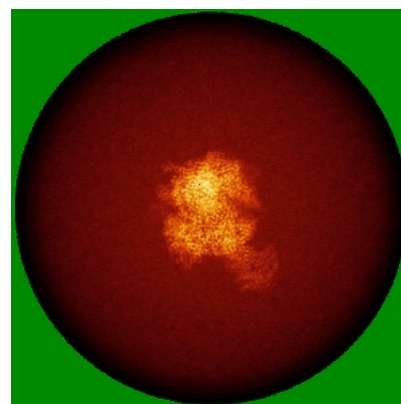
6.4.1 Primary map



X

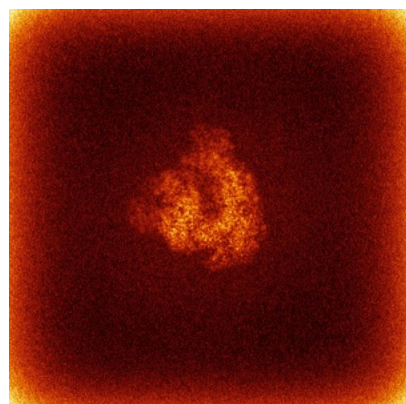


Y

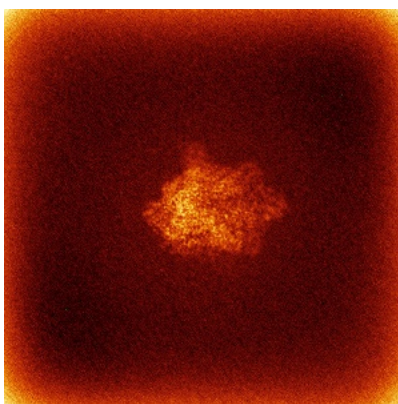


Z

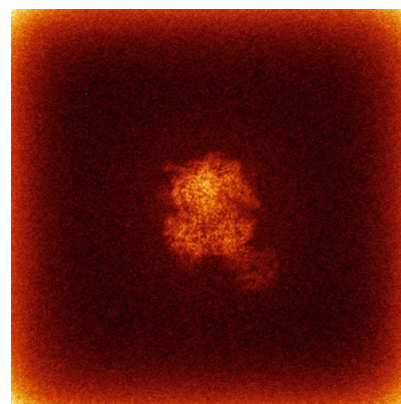
6.4.2 Raw map



X



Y

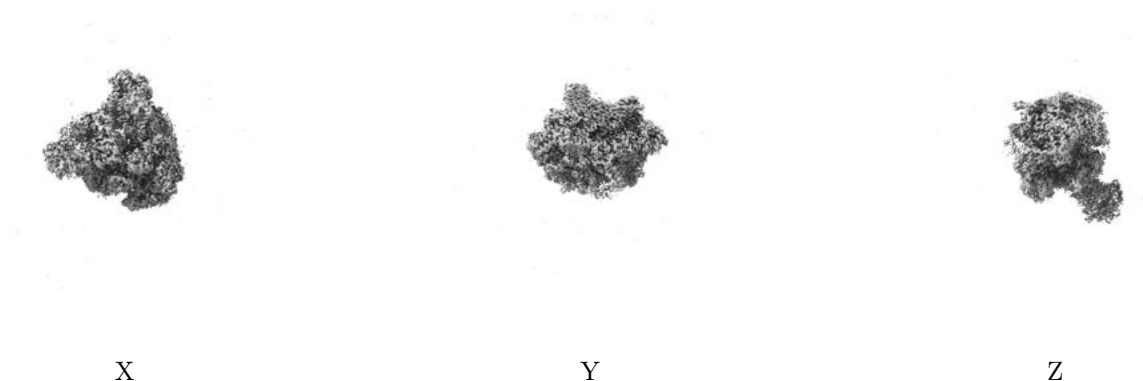


Z

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

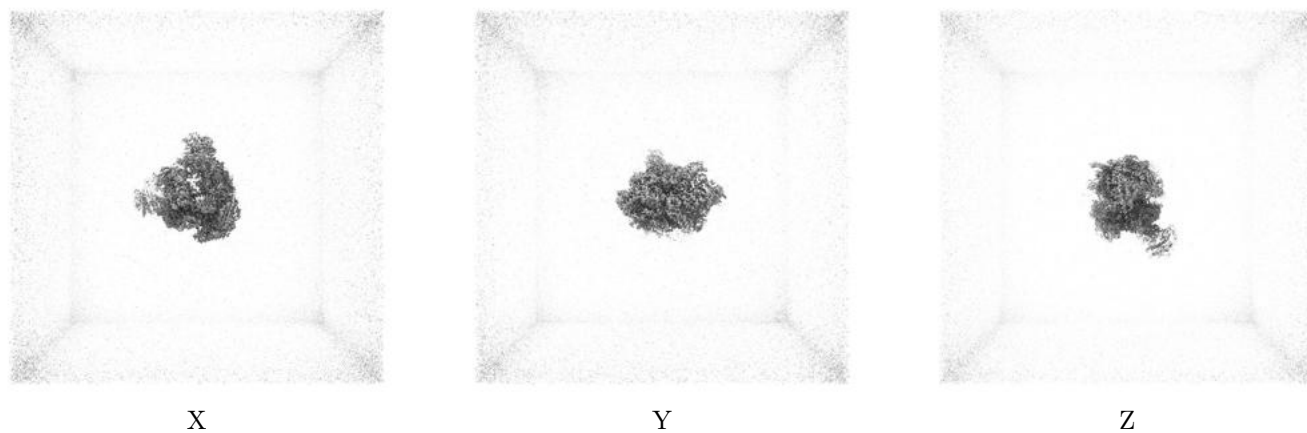
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

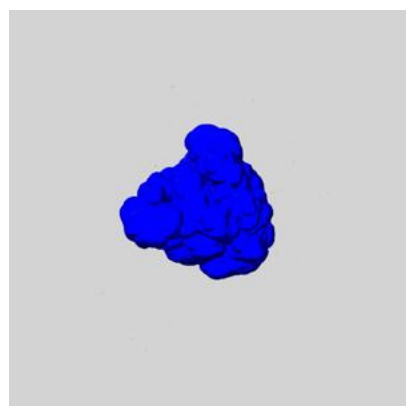
6.6 Mask visualisation [i](#)

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

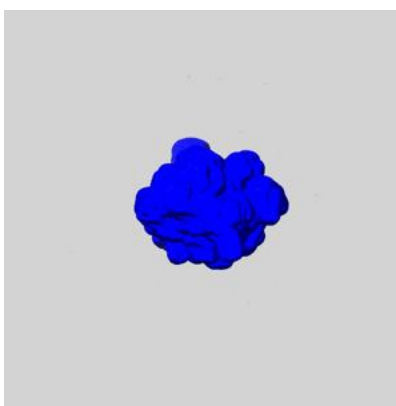
A mask typically either:

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

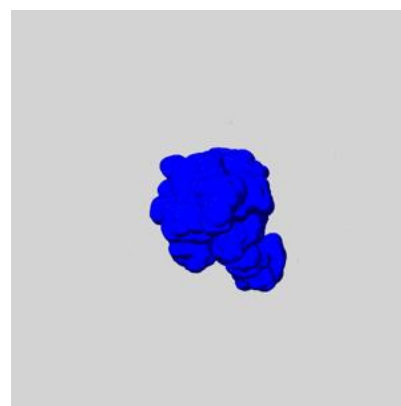
6.6.1 emd_38760_msk_1.map [i](#)



X



Y

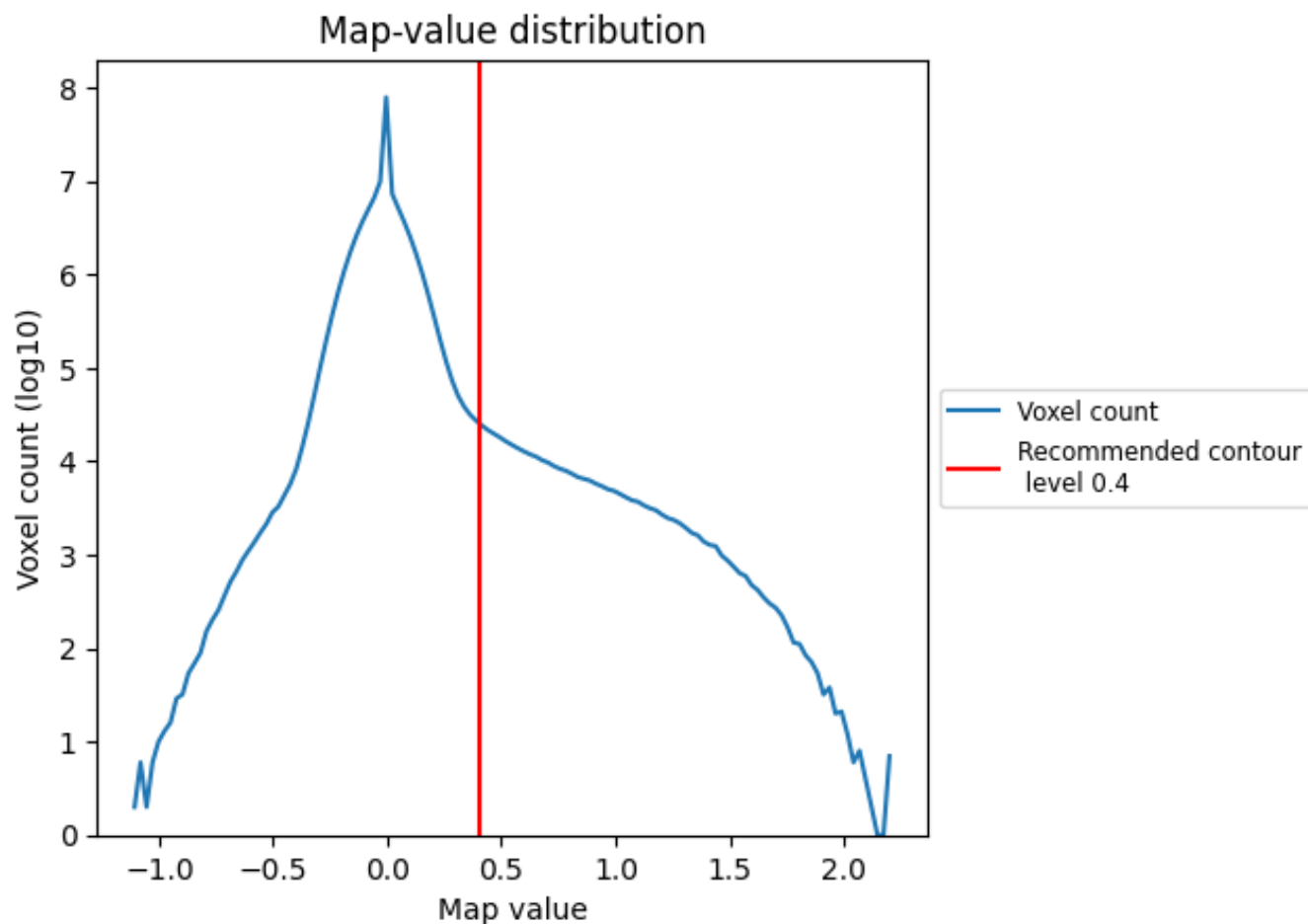


Z

7 Map analysis [i](#)

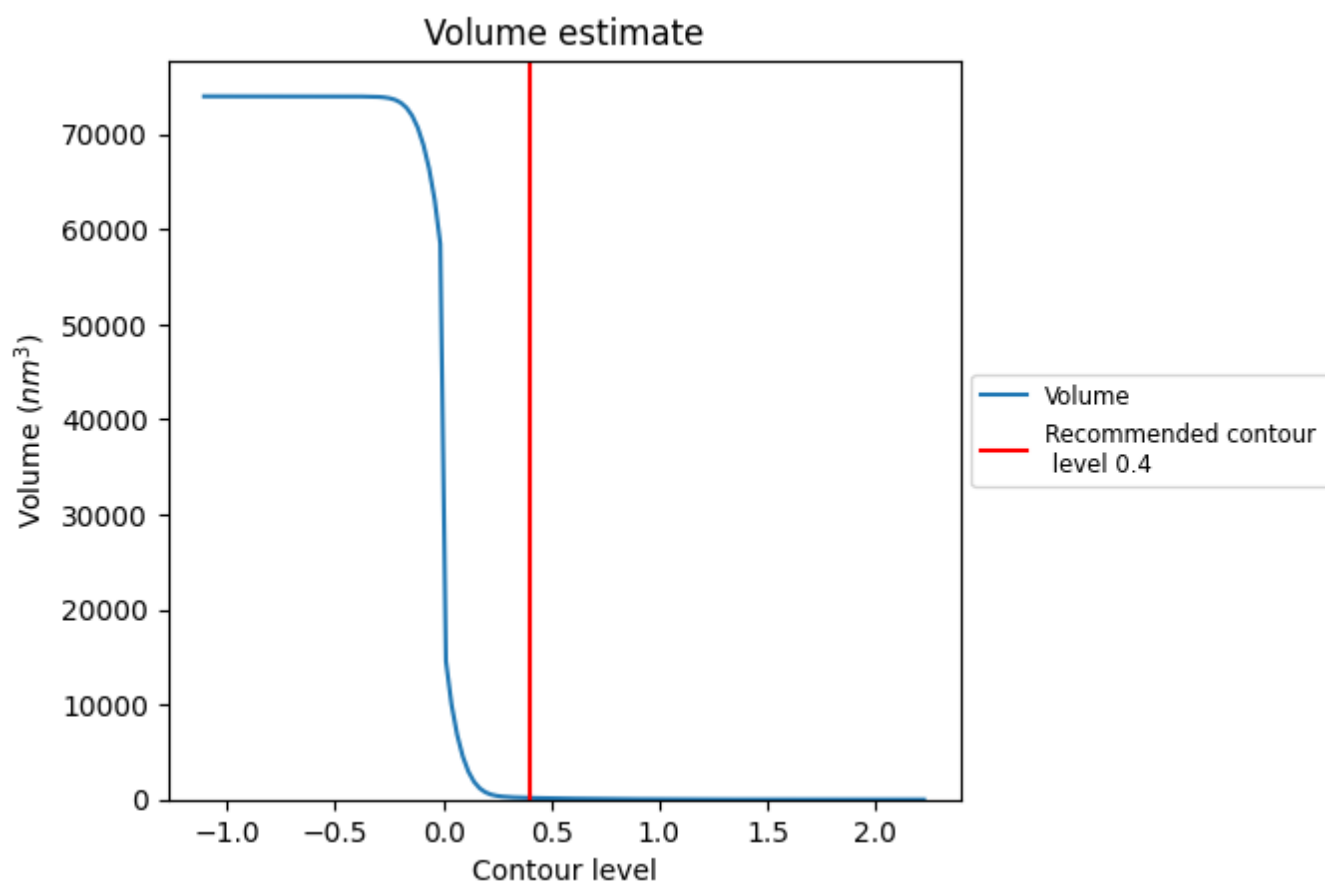
This section contains the results of statistical analysis of the map.

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.

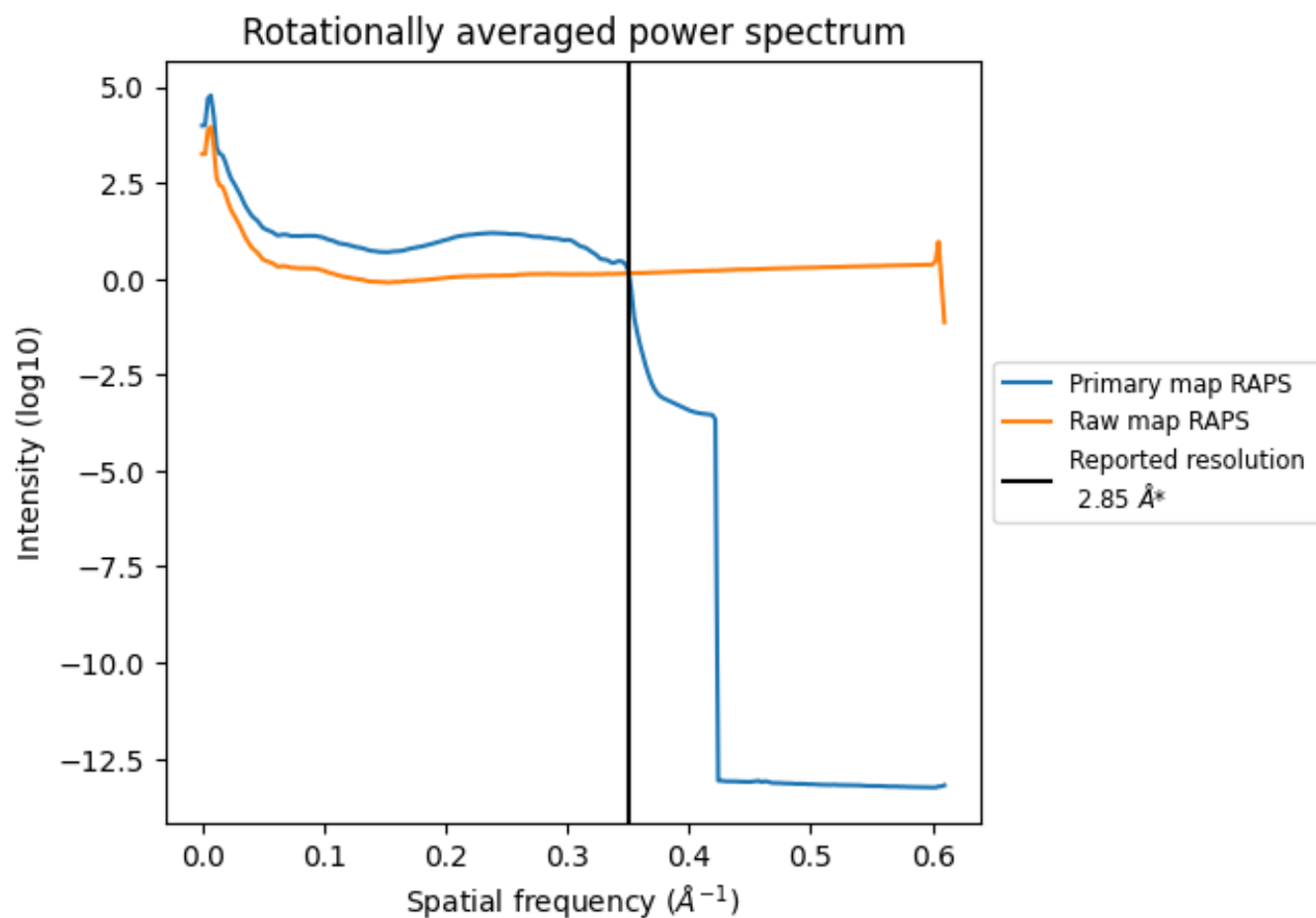
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179 nm³; this corresponds to an approximate mass of 162 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 ⓘ

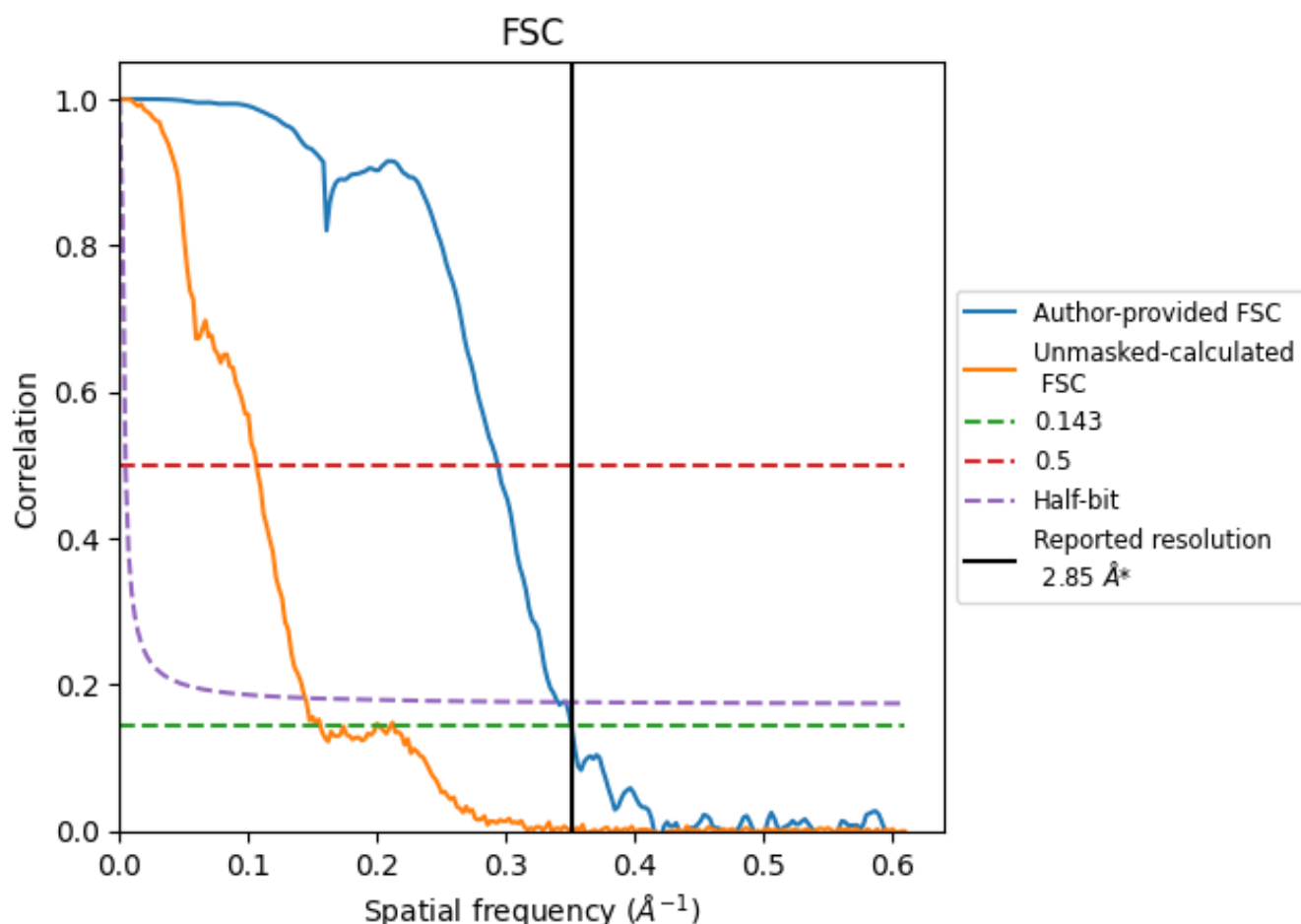


*Reported resolution corresponds to spatial frequency of 0.351 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

8.2 Resolution estimates [i](#)

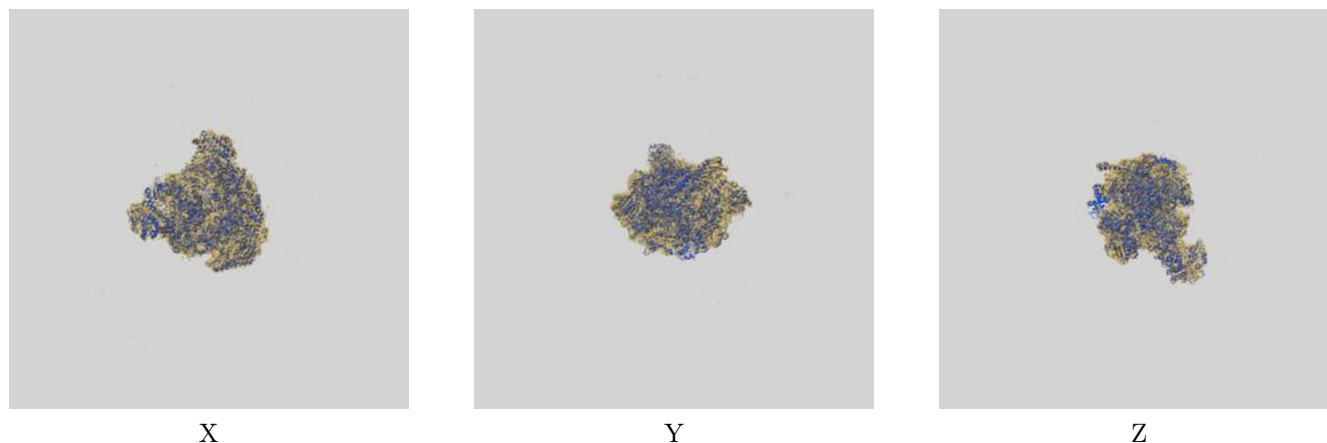
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.41	2.94
Unmasked-calculated*	6.41	9.40	6.93

*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 6.41 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

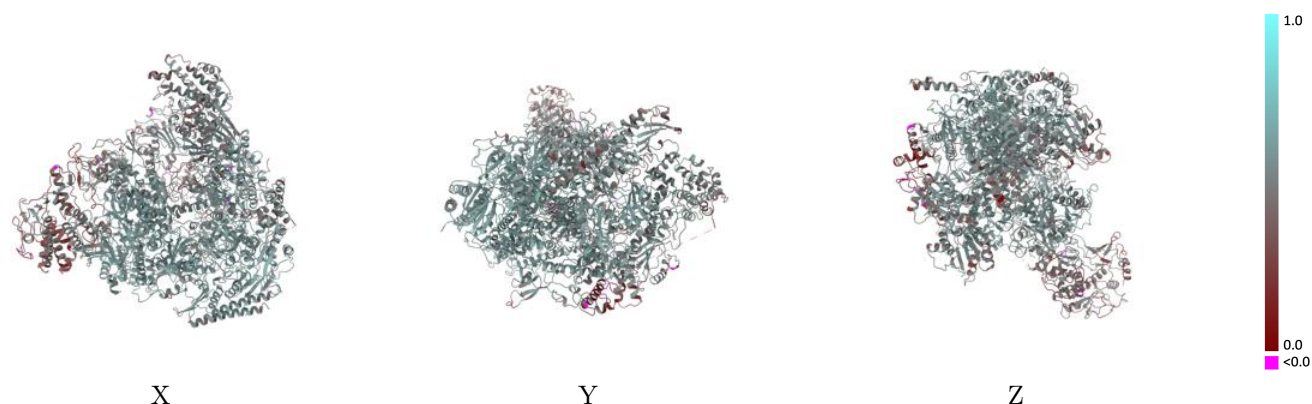
This section contains information regarding the fit between EMDB map EMD-38760 and PDB model 8XXT. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



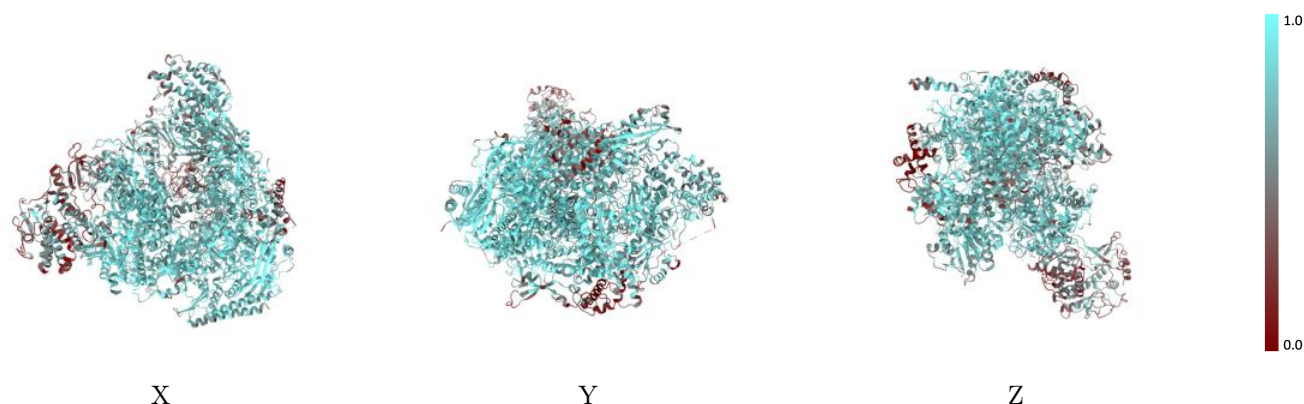
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



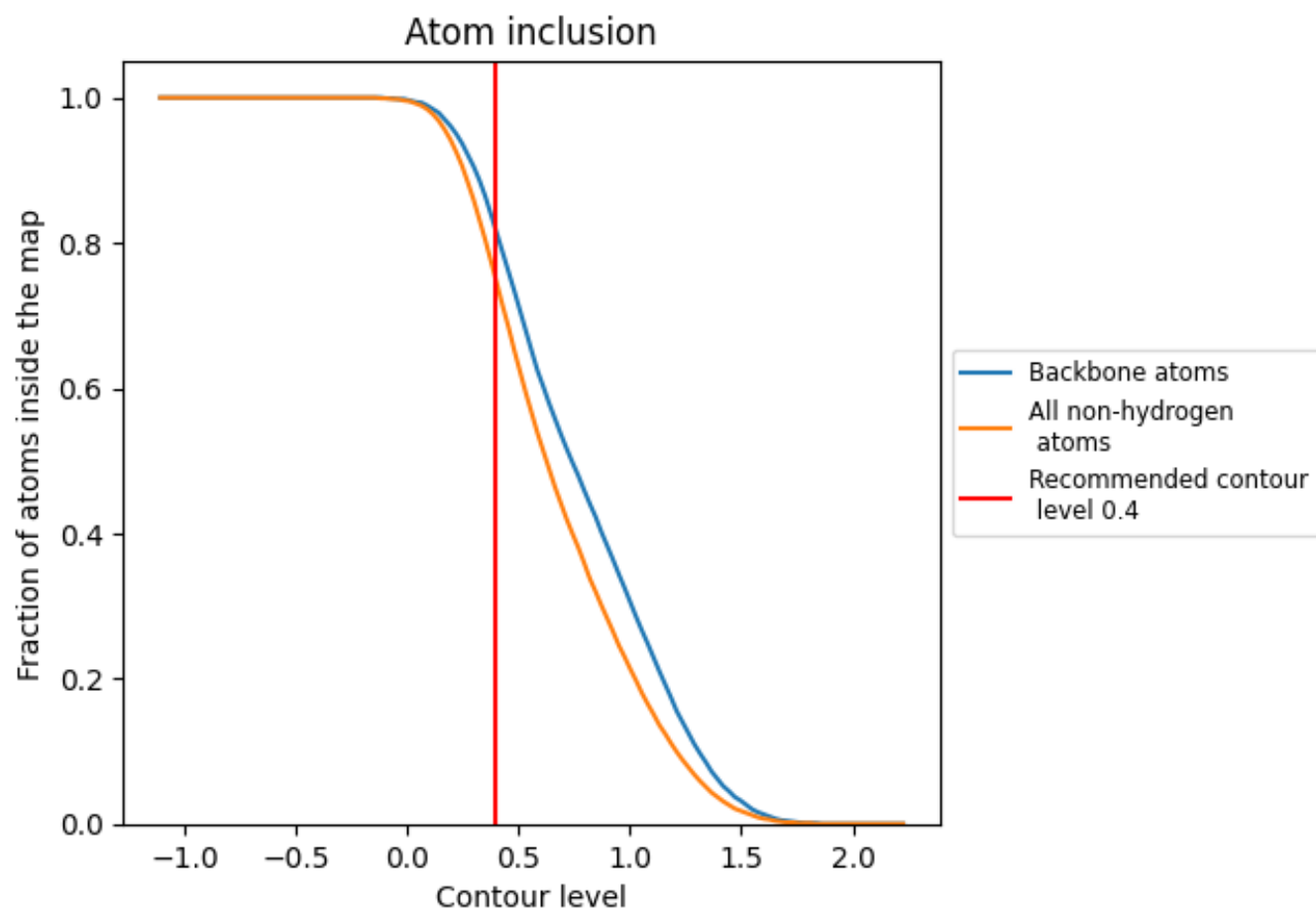
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 75% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7480	<div></div> 0.5250
A	<div></div> 0.8320	<div></div> 0.5600
B	<div></div> 0.8140	<div></div> 0.5490
C	<div></div> 0.8440	<div></div> 0.5700
D	<div></div> 0.7550	<div></div> 0.5130
E	<div></div> 0.7370	<div></div> 0.5400
F	<div></div> 0.5570	<div></div> 0.4370
G	<div></div> 0.7750	<div></div> 0.5230
H	<div></div> 0.8730	<div></div> 0.5620
I	<div></div> 0.4670	<div></div> 0.4200

1.0

0.0

<0.0