



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 06:50 pm GMT

PDB ID : 5OIK
EMDB ID : EMD-3817
Title : Structure of an RNA polymerase II-DSIF transcription elongation complex
Authors : Bernecky, C.; Plitzko, J.M.; Cramer, P.
Deposited on : 2017-07-18
Resolution : 3.70 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:

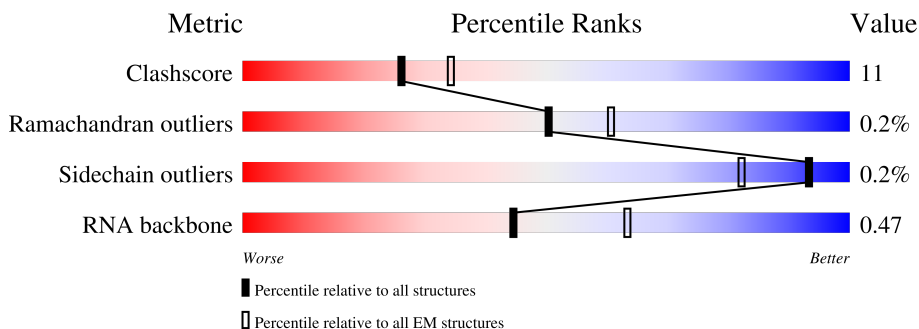
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.70 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.











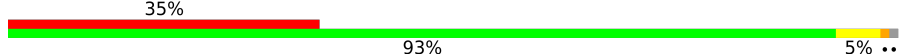

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1970	
2	B	1174	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	

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Mol	Chain	Length	Quality of chain
8	H	150	 71% 27% ..
9	I	125	 68% 25% • 6%
10	J	67	 72% 28%
11	K	117	 81% 16% ..
12	L	58	 50% 28% 22%
13	N	43	 12% 79% 19% •
14	P	50	 20% 14% 6% 60%
15	T	43	 5% 72% 26% •
16	Y	117	 35% 93% 5% ..
17	Z	1087	 8% 37% 7% 55%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 37988 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1421	11261	7084	2015	2090	72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1147	9142	5780	1612	1686	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	259	2079	1305	357	411	6	0	0

- Molecule 4 is a protein called Polymerase (RNA) II (DNA directed) polypeptide D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1008	635	170	199	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1711	1084	300	319	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	658	419	113	121	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1341	871	218	244	8	0	0

- Molecule 8 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	148	1186	750	194	237	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	117	946	584	169	182	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	67	533	345	90	92	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	920	593	152	173	2	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	45	379	236	73	64	6	0	0

- Molecule 13 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	N	43	709	335	130	202	42	0	9

- Molecule 14 is a RNA chain called RNA (5'-R(P*UP*AP*UP*AP*UP*AP*CP*AP*UP*A

P*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	P	20	427	192	80	135	20	0	0

- Molecule 15 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	T	43	874	419	157	256	42	0	0

- Molecule 16 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Y	116	911	570	159	173	9	0	0

- Molecule 17 is a protein called Transcription elongation factor SPT5.

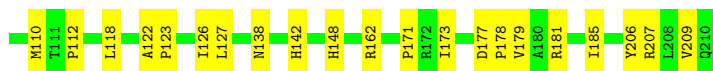
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Z	488	3894	2475	686	716	17	0	0

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

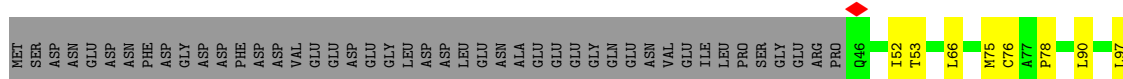
Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	I	2	Total	Zn	0
			2	2	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	
18	Y	1	Total	Zn	0
			1	1	

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

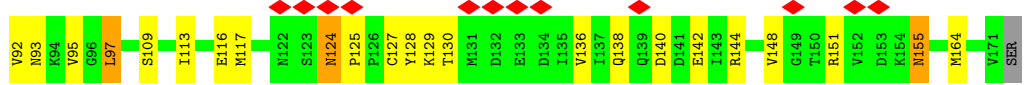
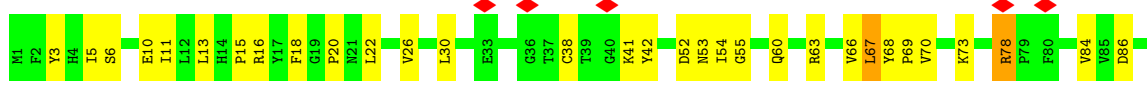
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	



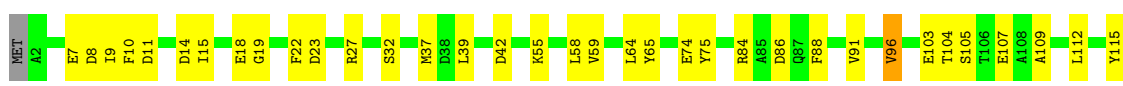
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



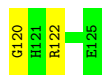
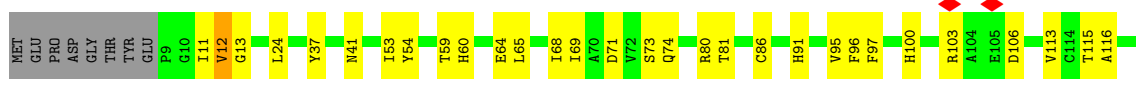
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: Uncharacterized protein



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

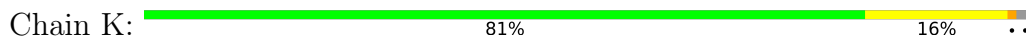


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

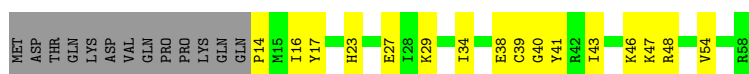




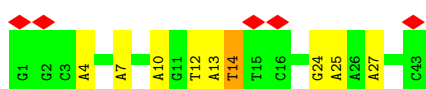
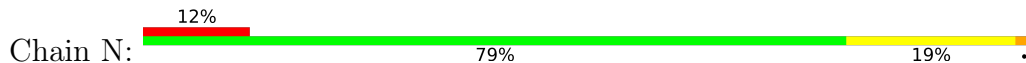
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: DNA (43-MER)



- Molecule 14: RNA (5'-R(P*UP*AP*UP*AP*UP*AP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3')



- Molecule 15: DNA (43-MER)



- Molecule 16: Transcription elongation factor SPT4



- Molecule 17: Transcription elongation factor SPT5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101140	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 ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.053	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.52	1/11467 (0.0%)	0.57	1/15479 (0.0%)
2	B	0.59	0/9325	0.60	1/12589 (0.0%)
3	C	0.64	0/2122	0.59	0/2883
4	D	0.29	0/1022	0.53	0/1377
5	E	0.50	0/1742	0.54	0/2353
6	F	0.55	0/668	0.56	0/903
7	G	0.34	0/1372	0.71	3/1861 (0.2%)
8	H	0.60	0/1207	0.57	0/1628
9	I	0.45	0/968	0.52	0/1311
10	J	0.68	0/542	0.64	0/730
11	K	0.54	0/939	0.56	1/1271 (0.1%)
12	L	0.61	0/385	0.54	0/511
13	N	0.78	0/785	1.28	4/1209 (0.3%)
14	P	0.66	0/478	0.74	0/742
15	T	0.92	1/979 (0.1%)	1.20	0/1508
16	Y	0.60	1/927 (0.1%)	0.67	1/1250 (0.1%)
17	Z	0.66	0/3963	0.67	5/5339 (0.1%)
All	All	0.58	3/38891 (0.0%)	0.65	16/52944 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
16	Y	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	105	GLY	CA-C	10.69	1.69	1.51
15	T	30	DA	O3'-P	-6.03	1.53	1.61
1	A	988	TRP	CB-CG	-5.13	1.41	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	LEU	CA-CB-CG	-7.26	98.60	115.30
16	Y	104	ARG	N-CA-C	6.43	128.35	111.00
7	G	78	ARG	NE-CZ-NH1	-6.38	117.11	120.30
2	B	526	LEU	CA-CB-CG	6.23	129.63	115.30
17	Z	450	ILE	N-CA-C	-6.23	94.18	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	910	LYS	Peptide
16	Y	105	GLY	Mainchain

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	11261	0	11390	302	0
2	B	9142	0	9157	288	0
3	C	2079	0	2032	64	0
4	D	1008	0	970	18	0
5	E	1711	0	1733	41	0
6	F	658	0	686	15	0
7	G	1341	0	1348	43	0
8	H	1186	0	1147	37	0
9	I	946	0	881	24	0
10	J	533	0	553	15	0
11	K	920	0	942	18	0
12	L	379	0	386	16	0
13	N	709	0	387	11	0
14	P	427	0	216	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	T	874	0	487	14	0
16	Y	911	0	904	5	0
17	Z	3894	0	3957	86	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
18	Y	1	0	0	0	0
19	A	1	0	0	0	0
All	All	37988	0	37176	841	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 841 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:LYS:NZ	17:Z:250:TRP:CE3	2.09	1.20
17:Z:417:GLU:OE2	17:Z:516:ARG:NH1	1.84	1.08
17:Z:471:TYR:O	17:Z:472:PHE:CG	2.23	0.90
2:B:888:THR:HG23	2:B:889:LYS:HG3	1.56	0.88
1:A:425:ASP:HB2	17:Z:583:PHE:CZ	2.08	0.87

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	1411/1970 (72%)	1353 (96%)	57 (4%)	1 (0%)	51 83
2	B	1143/1174 (97%)	1088 (95%)	55 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	255/275 (93%)	238 (93%)	17 (7%)	0	100	100
4	D	126/142 (89%)	113 (90%)	12 (10%)	1 (1%)	19	56
5	E	207/210 (99%)	197 (95%)	10 (5%)	0	100	100
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	162 (96%)	3 (2%)	4 (2%)	6	35
8	H	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
9	I	115/125 (92%)	105 (91%)	9 (8%)	1 (1%)	17	54
10	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
11	K	113/117 (97%)	113 (100%)	0	0	100	100
12	L	43/58 (74%)	40 (93%)	3 (7%)	0	100	100
16	Y	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
17	Z	480/1087 (44%)	463 (96%)	13 (3%)	4 (1%)	19	56
All	All	4467/5791 (77%)	4265 (96%)	191 (4%)	11 (0%)	50	78

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	18	PHE
7	G	124	ASN
4	D	91	LYS
9	I	12	VAL
17	Z	362	GLU

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	1252/1749 (72%)	1252 (100%)	0	100	100
2	B	996/1027 (97%)	996 (100%)	0	100	100
3	C	236/252 (94%)	236 (100%)	0	100	100
4	D	107/127 (84%)	105 (98%)	2 (2%)	57	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	189/190 (100%)	189 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	149/153 (97%)	147 (99%)	2 (1%)	69	83
8	H	129/131 (98%)	128 (99%)	1 (1%)	81	89
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	42/55 (76%)	42 (100%)	0	100	100
16	Y	102/103 (99%)	101 (99%)	1 (1%)	76	86
17	Z	429/940 (46%)	428 (100%)	1 (0%)	93	97
All	All	3967/5112 (78%)	3960 (100%)	7 (0%)	93	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	97	LEU
8	H	96	VAL
17	Z	338	ARG
16	Y	37	ASP
7	G	66	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	4	HIS
17	Z	519	GLN
9	I	22	ASN
16	Y	41	GLN
1	A	1360	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	19/50 (38%)	4 (21%)	1 (5%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	35	U
14	P	36	A
14	P	37	C
14	P	41	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	36	A

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](#)

Of 9 ligands modelled in this entry, 9 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	14:DT	O3'	15:DT	P	3.16

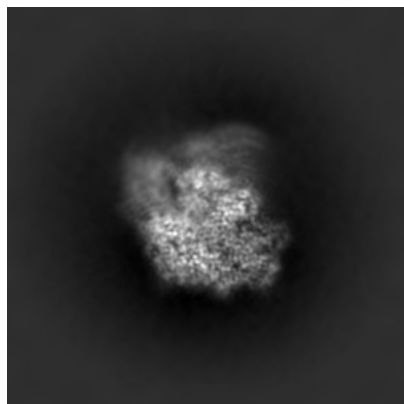
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3817. These allow visual inspection of the internal detail of the map and identification of artifacts.

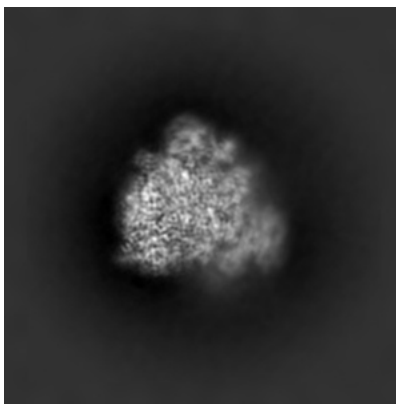
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

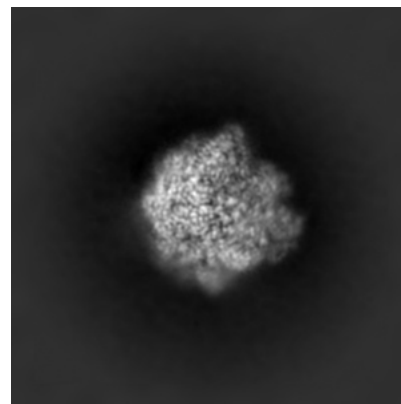
6.1.1 Primary map



X

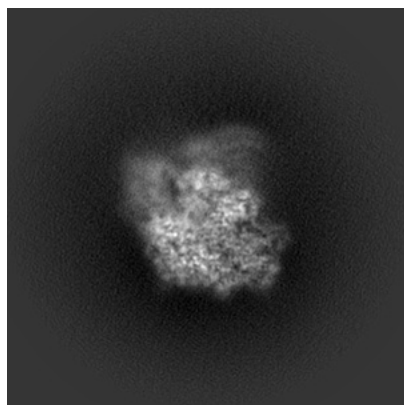


Y

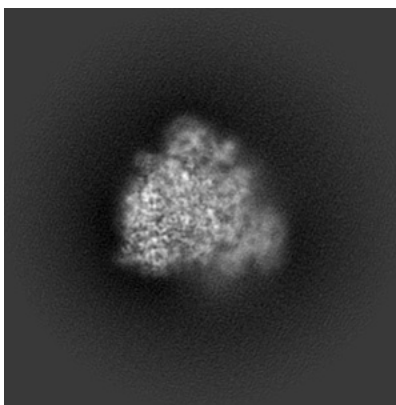


Z

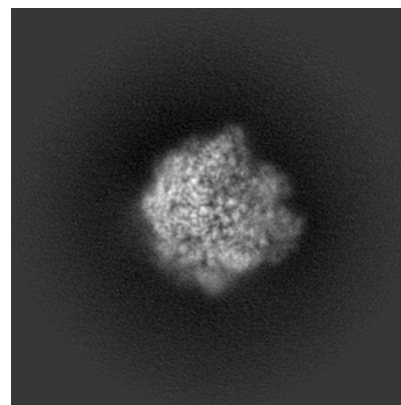
6.1.2 Raw map



X



Y

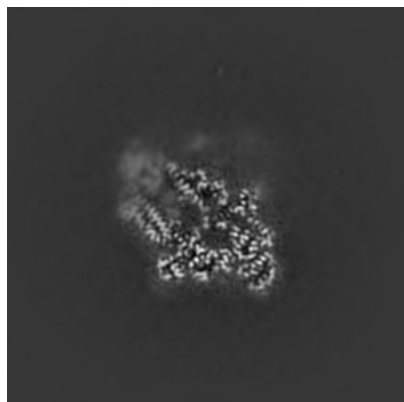


Z

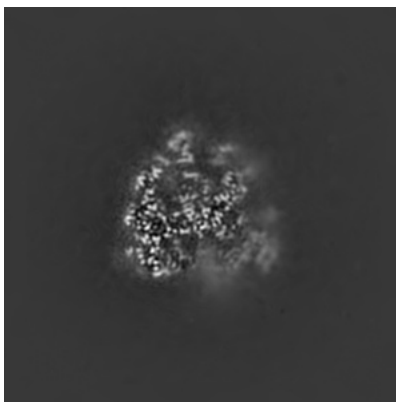
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

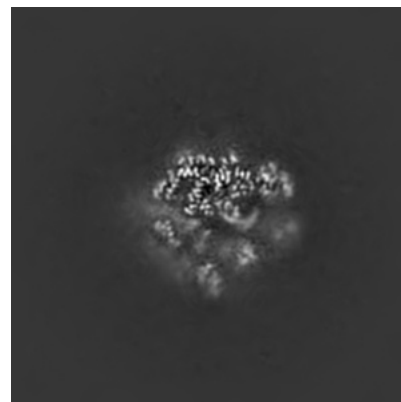
6.2.1 Primary map



X Index: 128

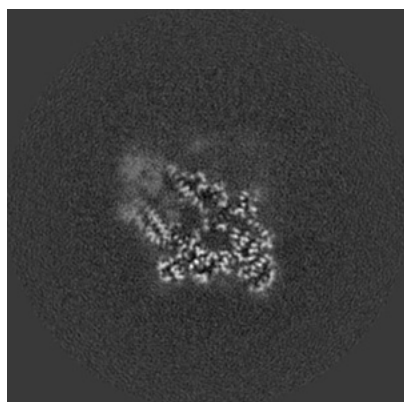


Y Index: 128

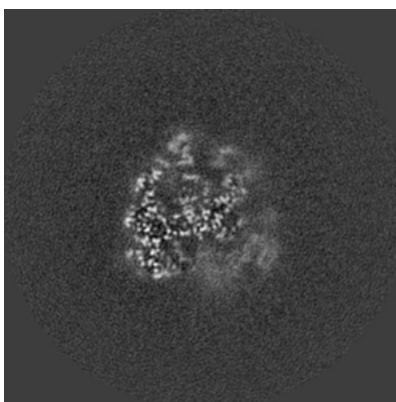


Z Index: 128

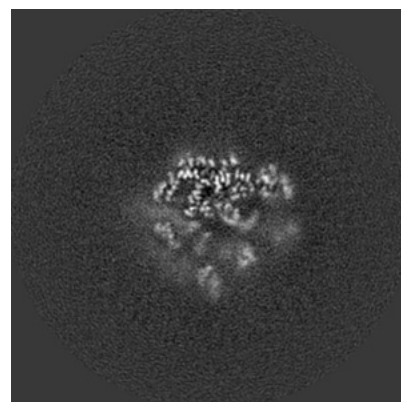
6.2.2 Raw map



X Index: 128



Y Index: 128

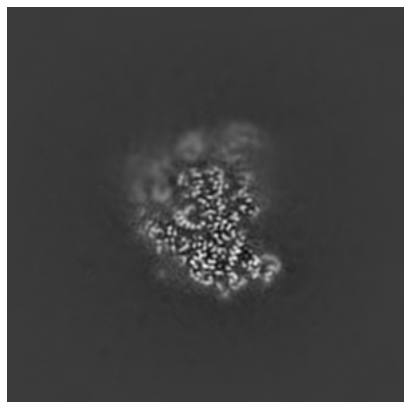


Z Index: 128

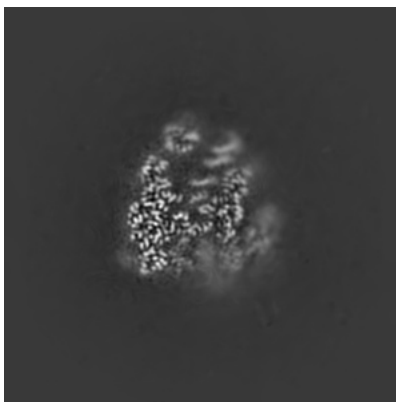
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

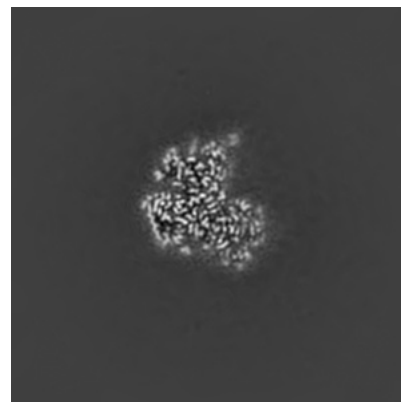
6.3.1 Primary map



X Index: 117

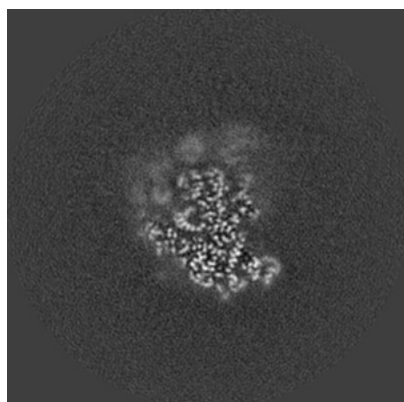


Y Index: 124

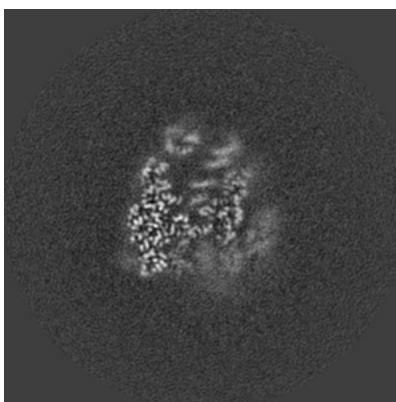


Z Index: 96

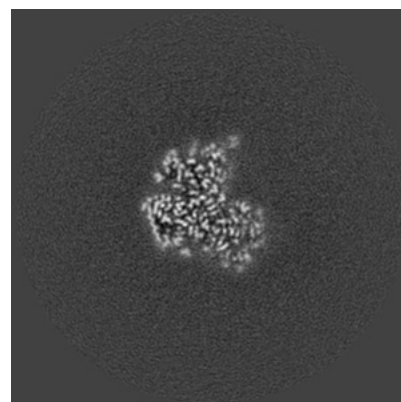
6.3.2 Raw map



X Index: 117



Y Index: 124

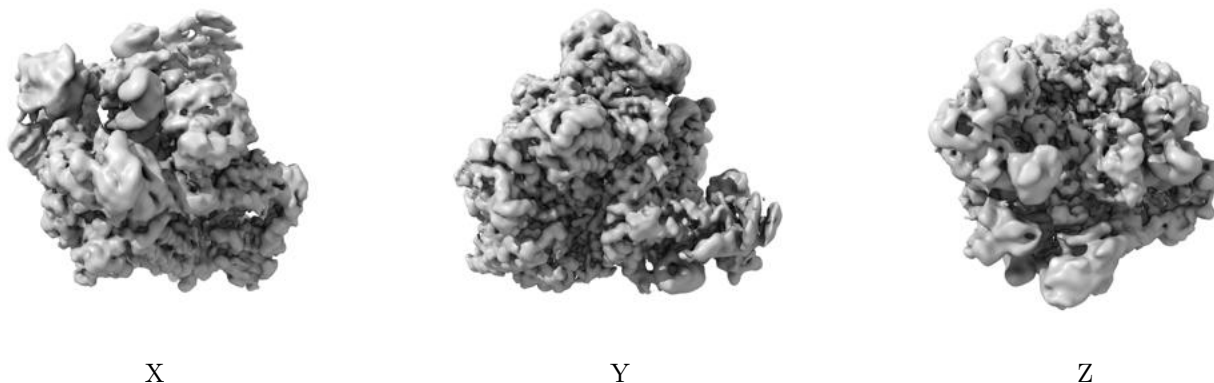


Z Index: 96

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

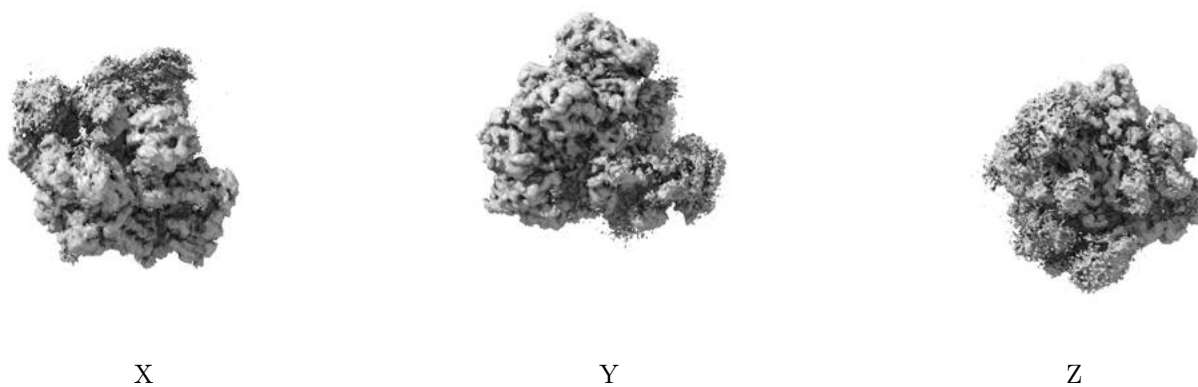
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

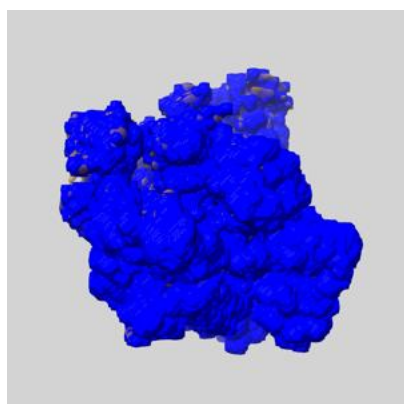
6.5 Mask visualisation [i](#)

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

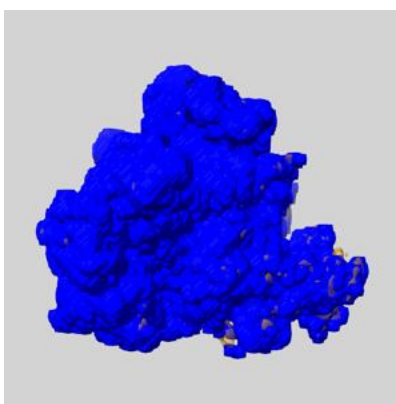
A mask typically either:

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

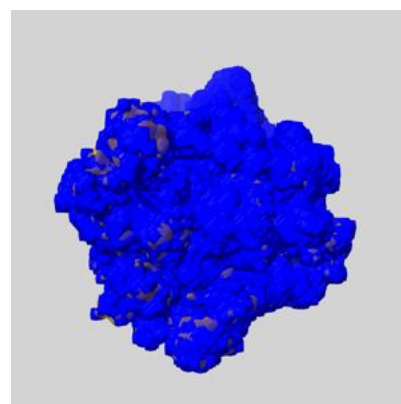
6.5.1 emd_3817_msk_1.map [i](#)



X



Y

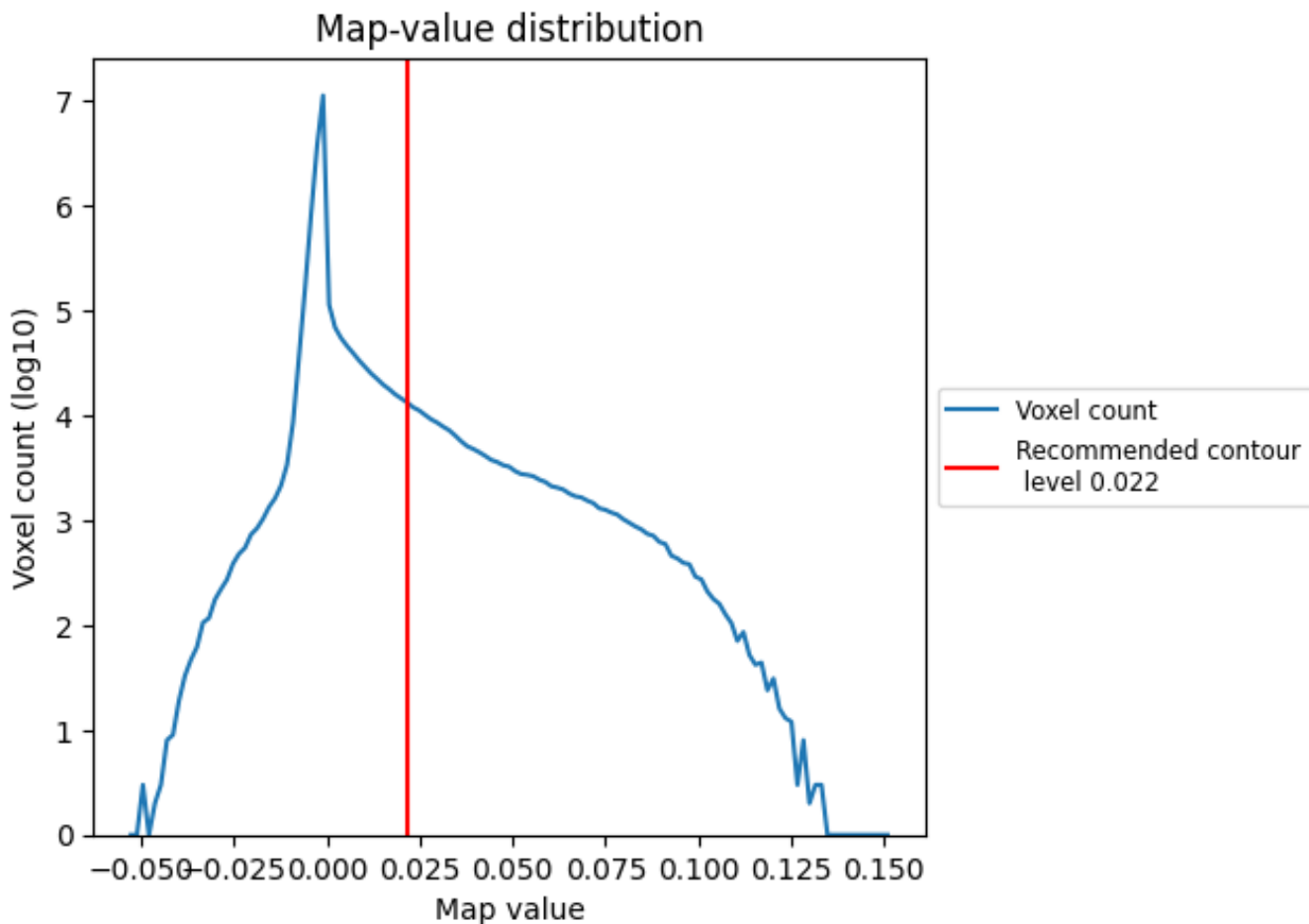


Z

7 Map analysis [i](#)

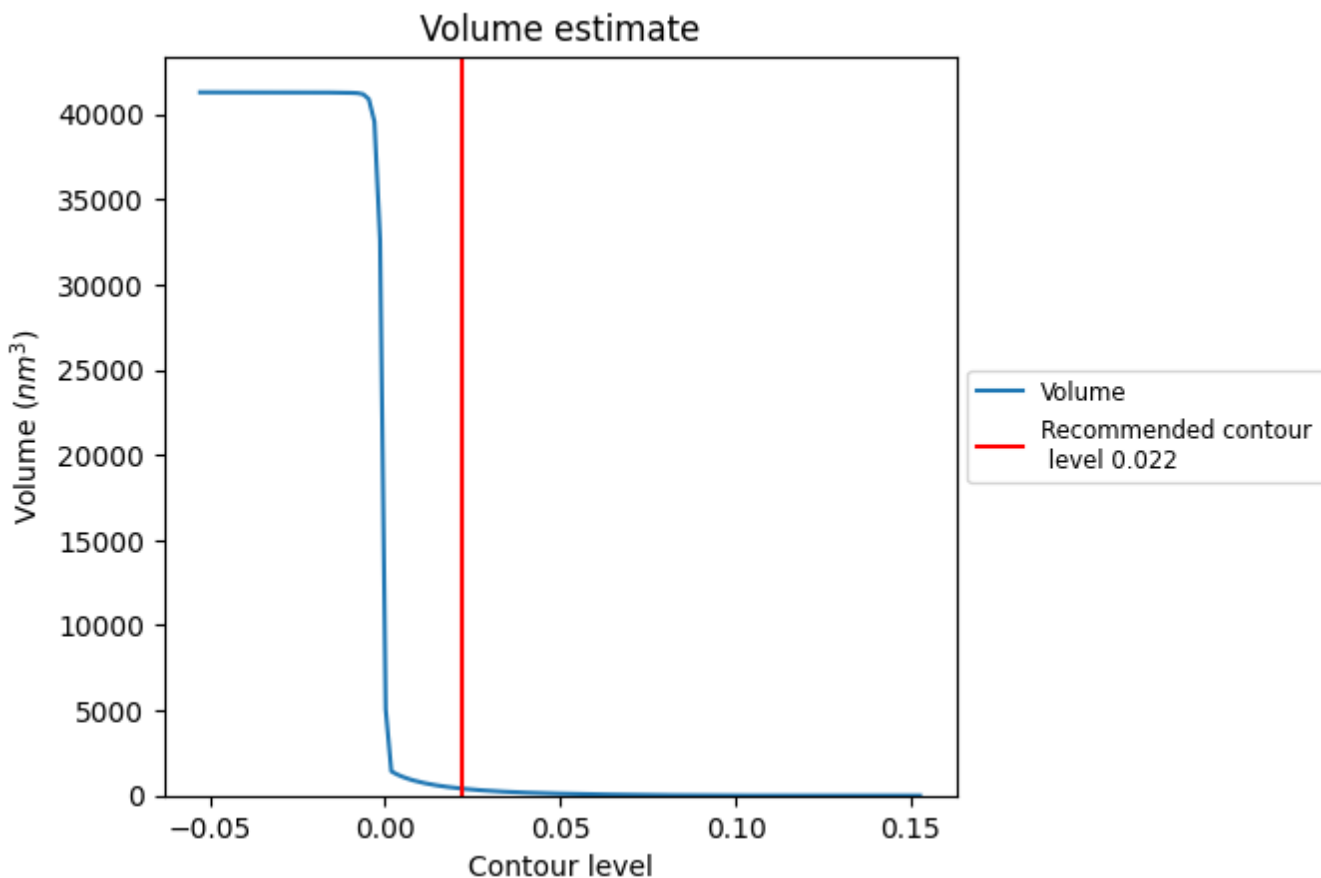
This section contains the results of statistical analysis of the map.

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.

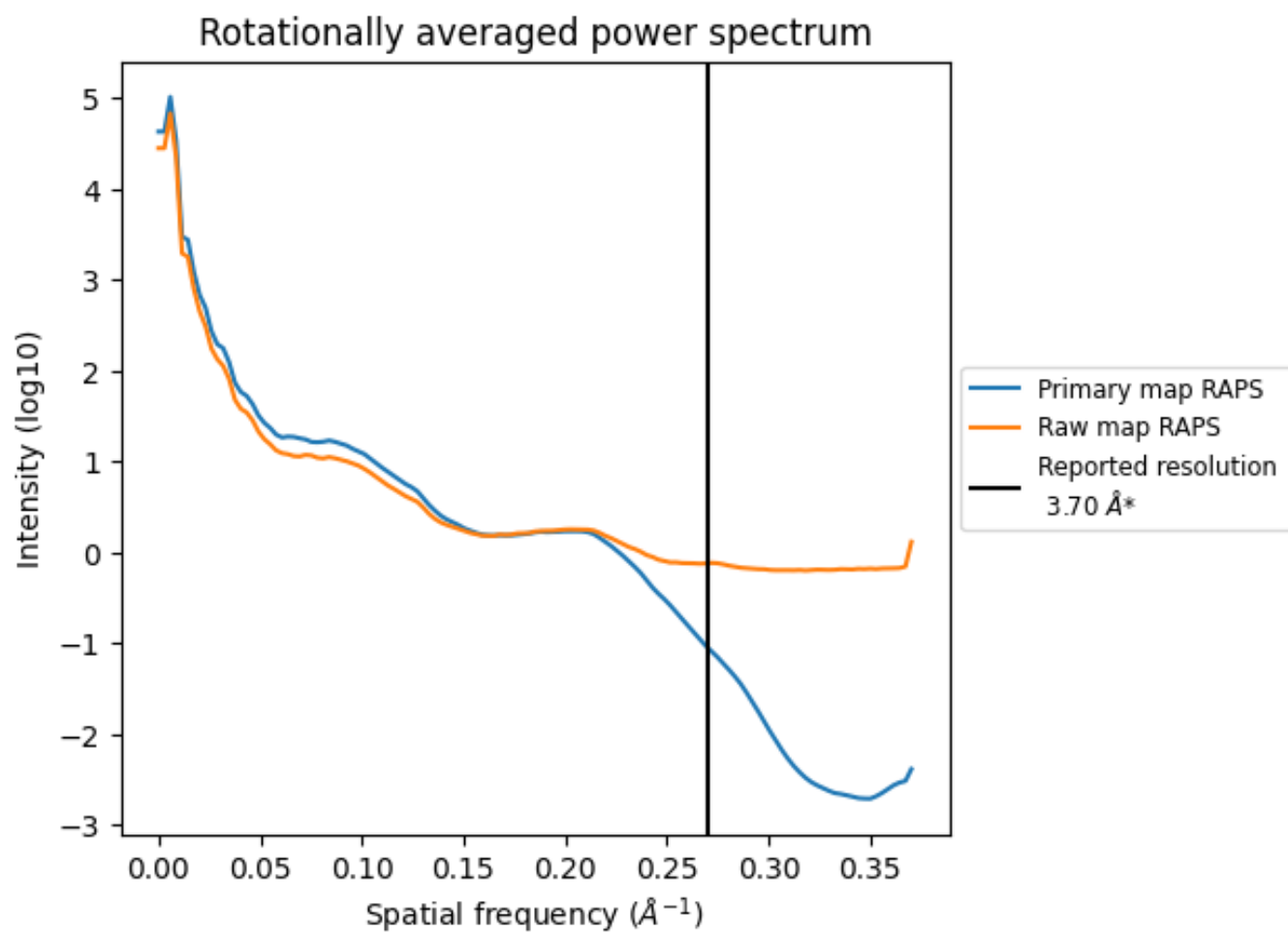
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 409 nm³; this corresponds to an approximate mass of 370 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

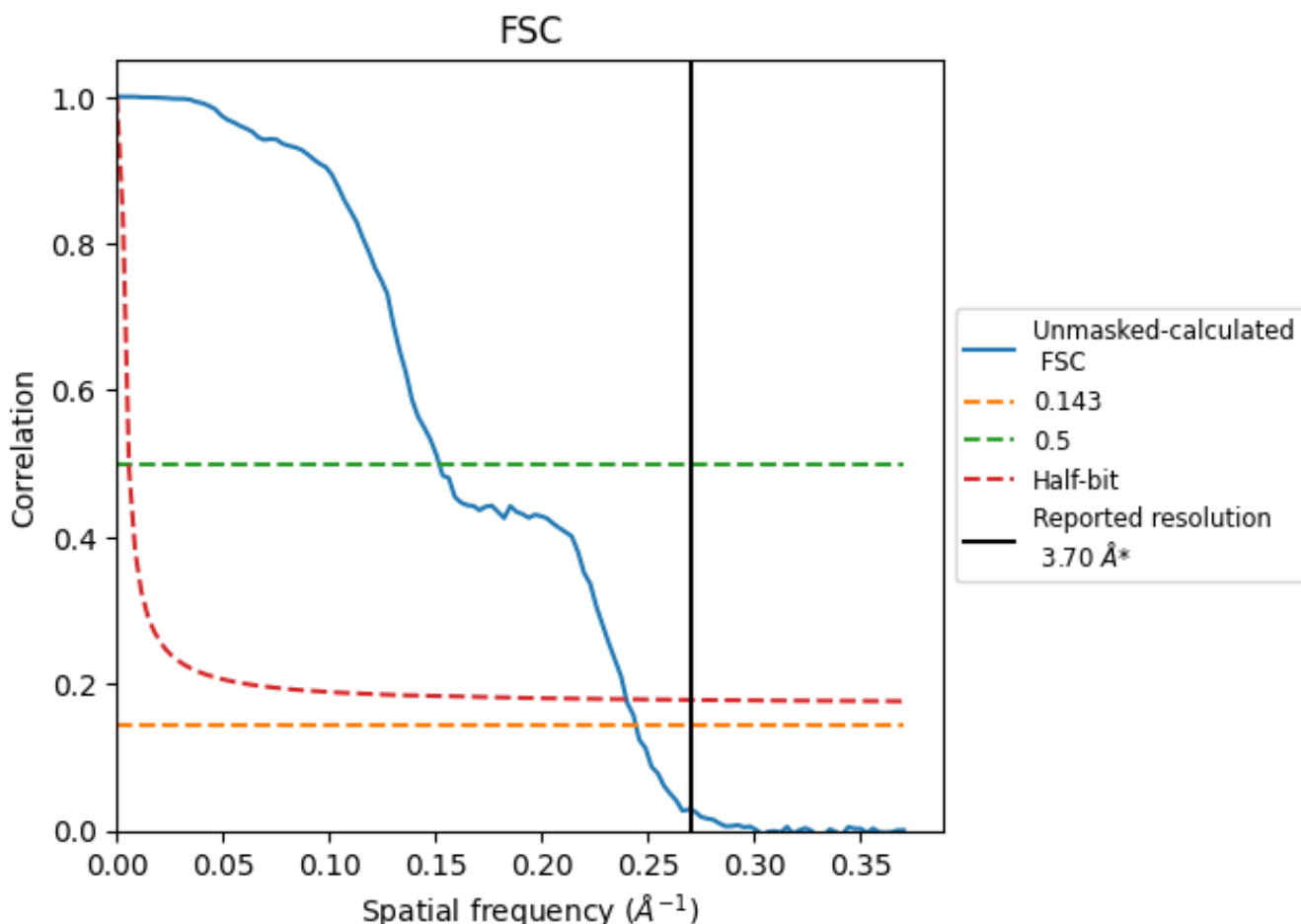


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

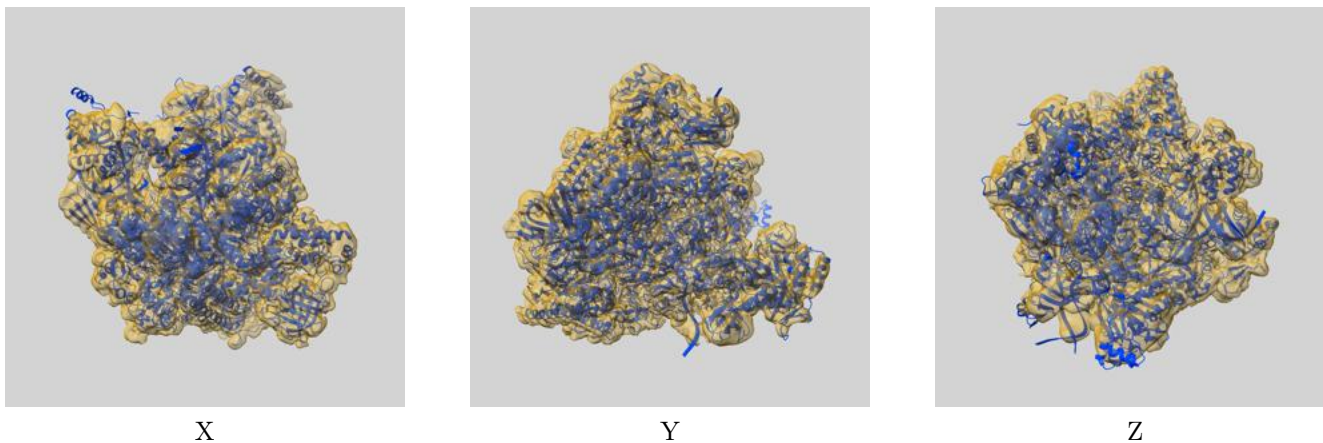
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	6.60	4.17

*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 4.09 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

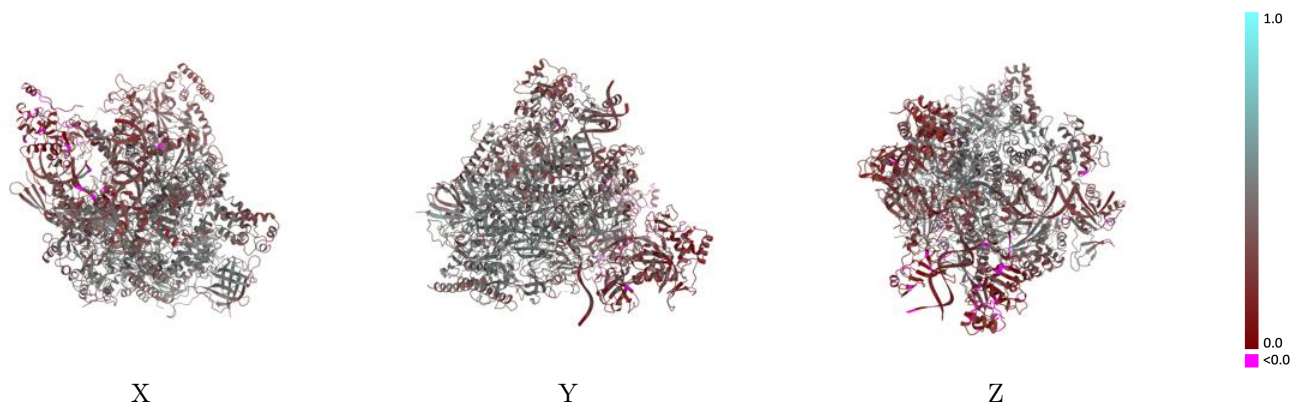
This section contains information regarding the fit between EMDB map EMD-3817 and PDB model 5OIK. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



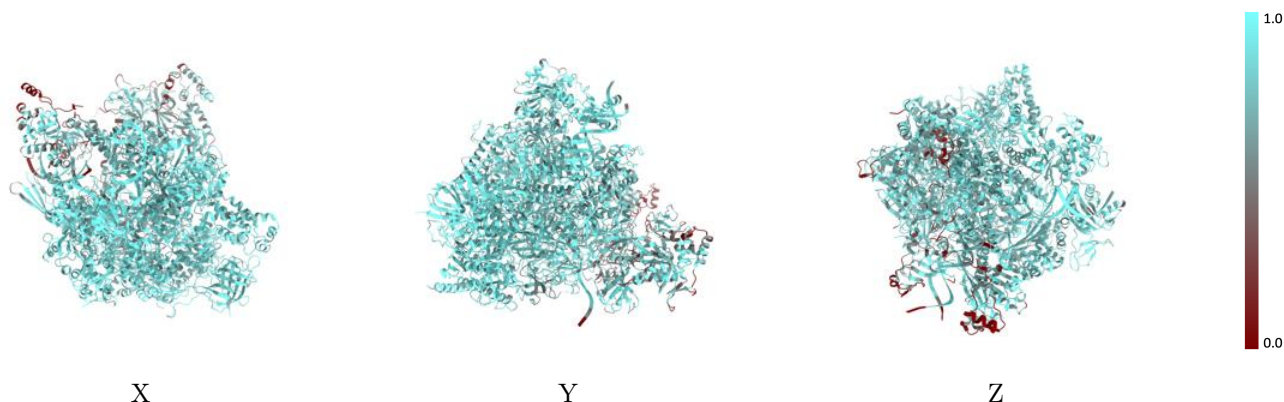
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



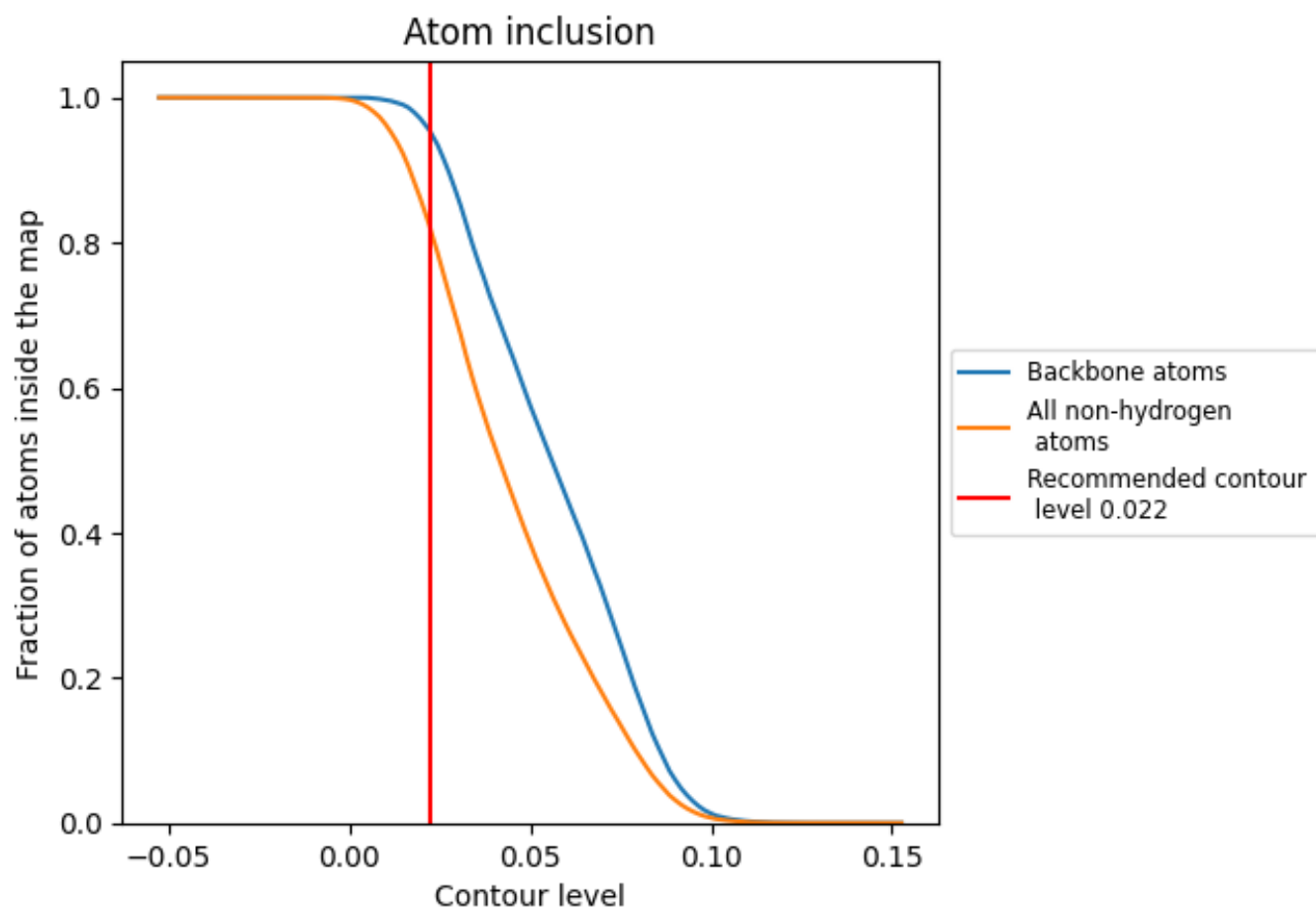
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 82% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8242	 0.3730
A	 0.8567	 0.4130
B	 0.8672	 0.4300
C	 0.9076	 0.4500
D	 0.5688	 0.2090
E	 0.8856	 0.3890
F	 0.8513	 0.4310
G	 0.7088	 0.2920
H	 0.8861	 0.4230
I	 0.8727	 0.3670
J	 0.8829	 0.4490
K	 0.8980	 0.4390
L	 0.8898	 0.4150
N	 0.8392	 0.2270
P	 0.8618	 0.3150
T	 0.8547	 0.2910
Y	 0.5354	 0.1090
Z	 0.6512	 0.2050

