



wwPDB EM Validation Summary Report ⓘ

Jul 11, 2023 – 02:12 pm BST

PDB ID : 8PKP
EMDB ID : EMD-17751
Title : Cryo-EM structure of the apo Anaphase-promoting complex/cyclosome (APC/C) at 3.2 Angstrom resolution
Authors : Hoefler, A.; Yu, J.; Chang, L.; Zhang, Z.; Yang, J.; Boland, A.; Barford, D.
Deposited on : 2023-06-27
Resolution : 3.20 Å(reported)
Based on initial model : 5G05

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:

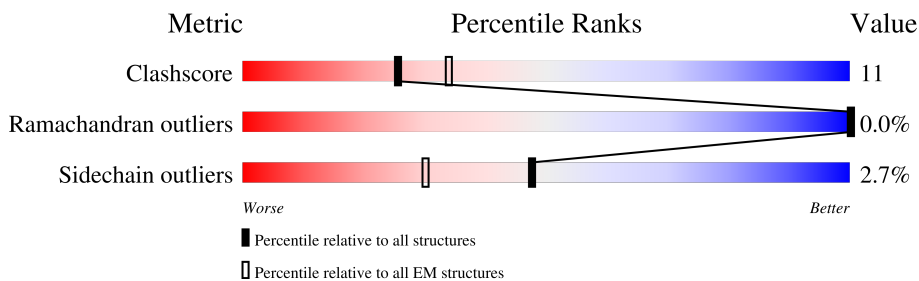
EMDB validation analysis : 0.0.1.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

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 3.20 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	1944	60% 21% 19%
2	D	121	40% 7% 54%
3	G	85	22% 9% 68%
3	W	85	25% 5% 71%
4	H	110	39% 12% 48%
5	J	824	42% 16% 42%
5	P	824	41% 17% 41%
6	K	620	65% 17% 17%

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Mol	Chain	Length	Quality of chain
6	Q	620	
7	L	185	
8	M	74	
9	O	755	
10	U	597	
10	V	597	
11	Y	565	
11	Z	565	
12	I	814	
13	N	822	
14	C	84	

2 Entry composition i

There are 15 unique types of molecules in this entry. The entry contains 64691 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1580	12311	7891	2074	2260	86	0	0

- Molecule 2 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	56	458	291	77	89	1	0	0

- Molecule 3 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	27	226	142	42	41	1	0	0
3	W	25	217	136	41	39	1	0	0

- Molecule 4 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	57	459	296	75	86	2	0	0

- Molecule 5 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	476	3601	2300	615	662	24	1	0
5	P	484	3883	2497	653	707	26	0	0

- Molecule 6 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	512	Total	C	N	O	S	0	0
			4134	2657	697	755	25		
6	Q	504	Total	C	N	O	S	0	0
			4049	2603	681	741	24		

- Molecule 7 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	179	Total	C	N	O	S	0	0
			1446	906	263	270	7		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	58	Total	C	N	O	S	0	0
			478	301	78	97	2		

- Molecule 9 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	683	Total	C	N	O	S	0	0
			5404	3444	941	993	26		

- Molecule 10 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	521	Total	C	N	O	S	0	0
			4221	2715	708	773	25		
10	V	534	Total	C	N	O	S	0	0
			4393	2826	740	802	25		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	499	Total	C	N	O	S	1	0
			3907	2471	681	728	27		
11	Z	486	Total	C	N	O	S	1	0
			3807	2413	664	705	25		

- Molecule 12 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	718	5722	3664	950	1074	34	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	809	GLU	-	expression tag	UNP Q9UJX5
I	810	ASN	-	expression tag	UNP Q9UJX5
I	811	LEU	-	expression tag	UNP Q9UJX5
I	812	TYR	-	expression tag	UNP Q9UJX5
I	813	PHE	-	expression tag	UNP Q9UJX5
I	814	GLN	-	expression tag	UNP Q9UJX5

- Molecule 13 is a protein called Anaphase-promoting complex subunit 2.

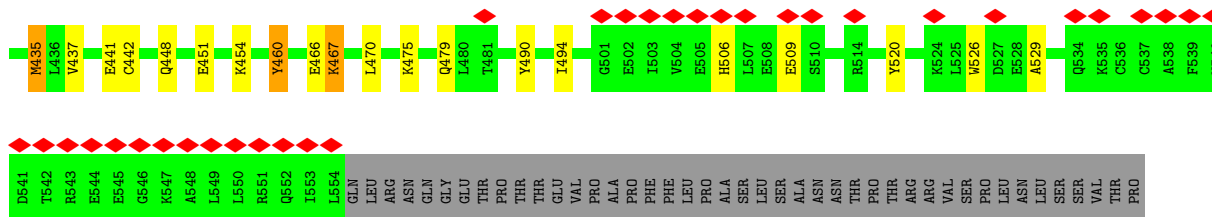
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	652	5294	3362	933	972	27	0	0

- Molecule 14 is a protein called Anaphase-promoting complex subunit 11.

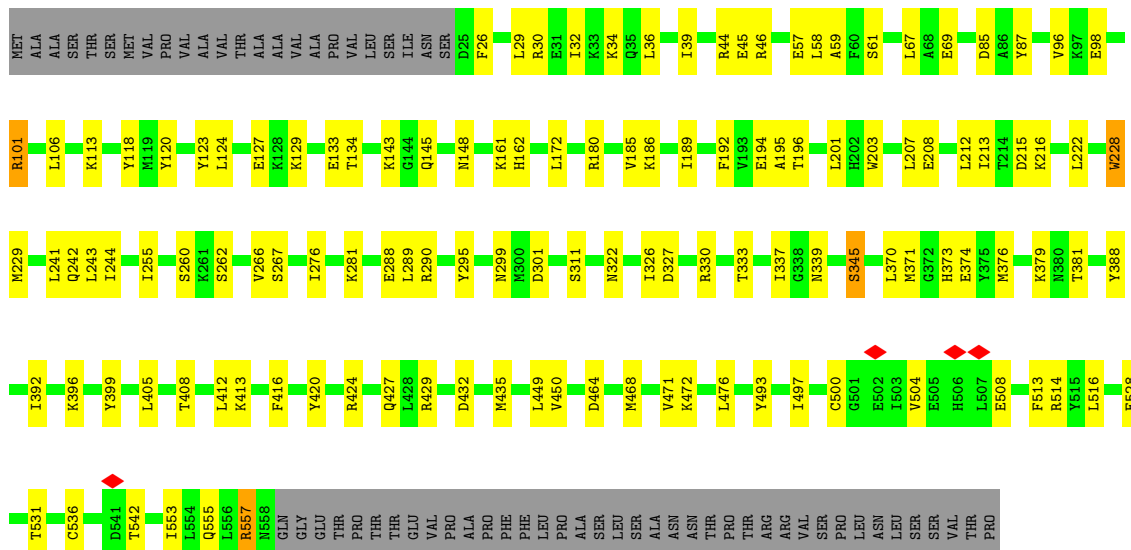
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C	84	680	431	123	110	16	0	0

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

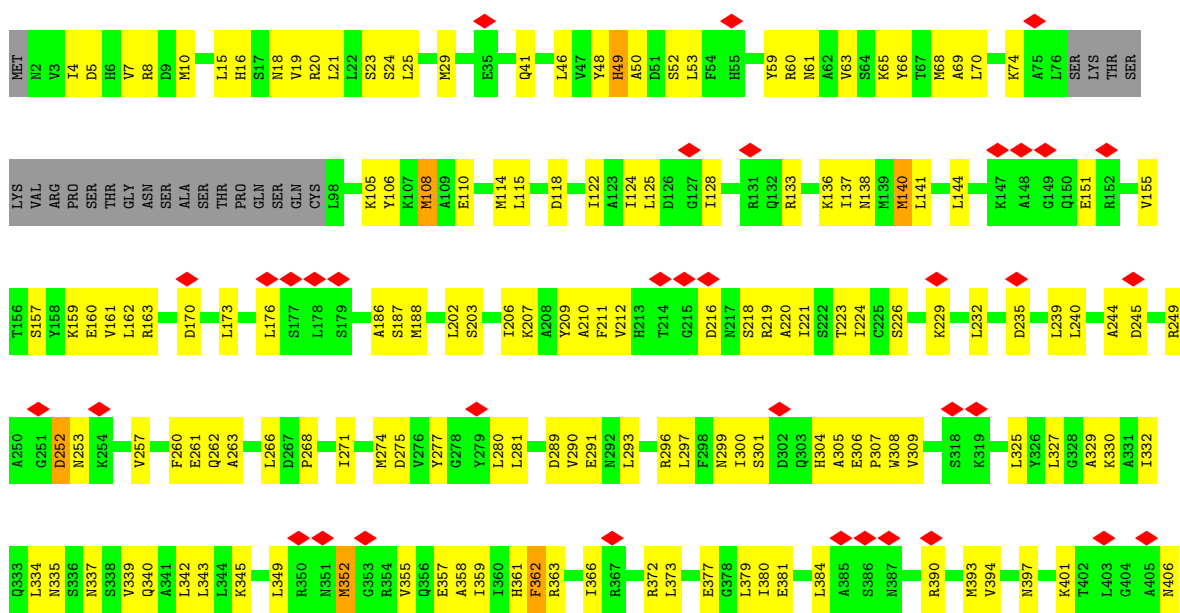
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
15	N	1	1	1	0

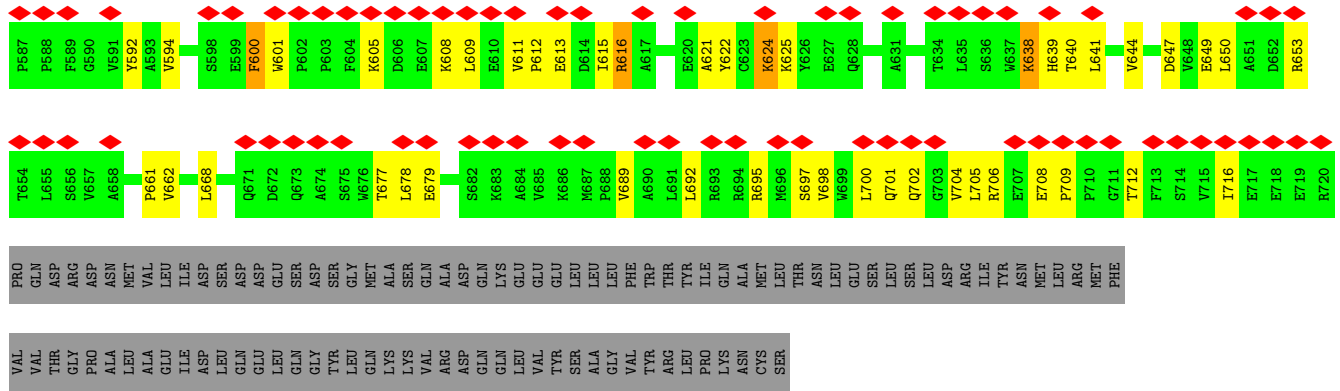


• Molecule 10: Cell division cycle protein 23 homolog

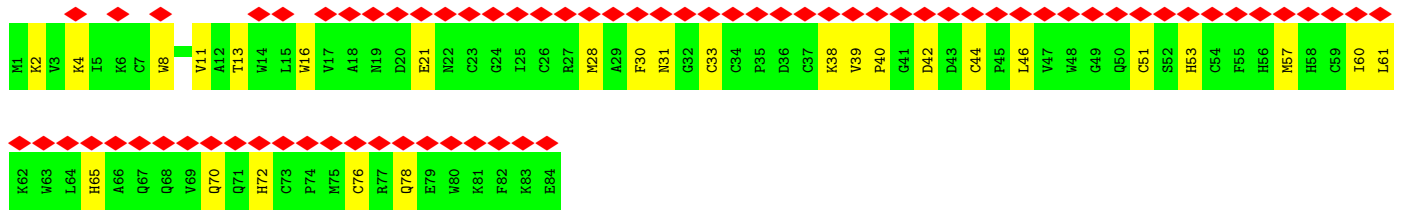
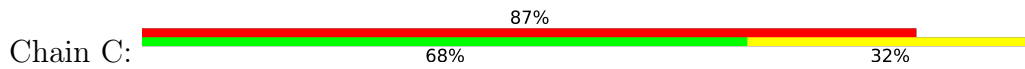


• Molecule 11: Anaphase-promoting complex subunit 7





● Molecule 14: Anaphase-promoting complex subunit 11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174356	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.975	Depositor
Minimum map value	-0.749	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.37	0/12594	0.53	0/17122
2	D	0.35	0/470	0.47	0/643
3	G	0.27	0/227	0.60	0/302
3	W	0.33	0/218	0.60	0/288
4	H	0.30	0/468	0.45	0/631
5	J	0.31	0/3686	0.50	0/5000
5	P	0.34	0/3975	0.48	0/5371
6	K	0.32	0/4233	0.47	0/5730
6	Q	0.34	0/4148	0.50	0/5620
7	L	0.32	0/1480	0.55	0/2005
8	M	0.29	0/486	0.52	0/658
9	O	0.36	0/5504	0.49	0/7435
10	U	0.32	0/4318	0.49	0/5839
10	V	0.37	0/4493	0.49	0/6065
11	Y	0.28	0/3970	0.55	0/5365
11	Z	0.28	0/3870	0.53	0/5233
12	I	0.31	0/5841	0.52	0/7909
13	N	0.28	0/5405	0.53	0/7315
14	C	0.23	0/703	0.42	0/951
All	All	0.33	0/66089	0.51	0/89482

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

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	12311	0	12224	277	0
2	D	458	0	434	9	0
3	G	226	0	233	10	0
3	W	217	0	231	3	0
4	H	459	0	449	12	0
5	J	3601	0	3314	100	0
5	P	3883	0	3834	115	0
6	K	4134	0	4060	75	0
6	Q	4049	0	3948	100	0
7	L	1446	0	1423	53	0
8	M	478	0	454	11	0
9	O	5404	0	5452	137	0
10	U	4221	0	4106	65	0
10	V	4393	0	4362	94	0
11	Y	3907	0	3975	165	0
11	Z	3807	0	3885	136	0
12	I	5722	0	5680	118	0
13	N	5294	0	5294	116	0
14	C	680	0	649	24	0
15	N	1	0	0	0	0
All	All	64691	0	64007	1461	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 1461 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)
9:O:443:GLN:HE22	12:I:514:PHE:H	1.22	0.86
5:P:12:ILE:HG21	5:P:43:LEU:HD21	1.57	0.86
11:Y:105:LYS:HA	11:Y:108:MET:HE3	1.57	0.85
1:A:1193:ILE:HG23	1:A:1208:LEU:HD21	1.62	0.80
5:J:160:GLU:HG3	5:J:161:LYS:HG2	1.63	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1546/1944 (80%)	1491 (96%)	53 (3%)	2 (0%)	51	83
2	D	54/121 (45%)	53 (98%)	1 (2%)	0	100	100
3	G	25/85 (29%)	25 (100%)	0	0	100	100
3	W	23/85 (27%)	23 (100%)	0	0	100	100
4	H	55/110 (50%)	55 (100%)	0	0	100	100
5	J	471/824 (57%)	458 (97%)	13 (3%)	0	100	100
5	P	480/824 (58%)	468 (98%)	11 (2%)	1 (0%)	47	79
6	K	506/620 (82%)	492 (97%)	14 (3%)	0	100	100
6	Q	500/620 (81%)	488 (98%)	12 (2%)	0	100	100
7	L	175/185 (95%)	163 (93%)	11 (6%)	1 (1%)	25	64
8	M	54/74 (73%)	51 (94%)	3 (6%)	0	100	100
9	O	675/755 (89%)	664 (98%)	11 (2%)	0	100	100
10	U	517/597 (87%)	506 (98%)	11 (2%)	0	100	100
10	V	532/597 (89%)	523 (98%)	9 (2%)	0	100	100
11	Y	496/565 (88%)	482 (97%)	14 (3%)	0	100	100
11	Z	483/565 (86%)	472 (98%)	11 (2%)	0	100	100
12	I	710/814 (87%)	692 (98%)	18 (2%)	0	100	100
13	N	644/822 (78%)	624 (97%)	20 (3%)	0	100	100
14	C	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
All	All	8028/10291 (78%)	7808 (97%)	216 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1393	MET
7	L	48	ASP

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Mol	Chain	Res	Type
5	P	703	PRO
1	A	832	HIS

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	1357/1720 (79%)	1320 (97%)	37 (3%)	44	75
2	D	52/115 (45%)	52 (100%)	0	100	100
3	G	24/77 (31%)	24 (100%)	0	100	100
3	W	24/77 (31%)	23 (96%)	1 (4%)	30	65
4	H	49/89 (55%)	48 (98%)	1 (2%)	55	80
5	J	343/727 (47%)	331 (96%)	12 (4%)	36	69
5	P	414/727 (57%)	399 (96%)	15 (4%)	35	69
6	K	439/548 (80%)	428 (98%)	11 (2%)	47	77
6	Q	425/548 (78%)	415 (98%)	10 (2%)	49	77
7	L	163/170 (96%)	156 (96%)	7 (4%)	29	64
8	M	52/67 (78%)	48 (92%)	4 (8%)	13	44
9	O	582/650 (90%)	566 (97%)	16 (3%)	44	75
10	U	434/520 (84%)	423 (98%)	11 (2%)	47	77
10	V	464/520 (89%)	453 (98%)	11 (2%)	49	77
11	Y	423/484 (87%)	411 (97%)	12 (3%)	43	74
11	Z	412/484 (85%)	401 (97%)	11 (3%)	44	75
12	I	638/736 (87%)	626 (98%)	12 (2%)	57	81
13	N	578/724 (80%)	564 (98%)	14 (2%)	49	77
14	C	75/75 (100%)	73 (97%)	2 (3%)	44	75
All	All	6948/9058 (77%)	6761 (97%)	187 (3%)	48	75

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	U	342	SER
11	Y	252	ASP
10	U	399	TYR
10	V	435	MET
11	Z	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
5	P	599	ASN
13	N	235	GLN
6	Q	179	GLN
12	I	584	HIS
11	Z	143	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](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

There are no chain breaks in this entry.

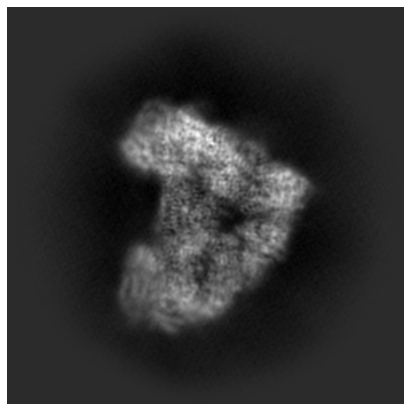
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17751. These allow visual inspection of the internal detail of the map and identification of artifacts.

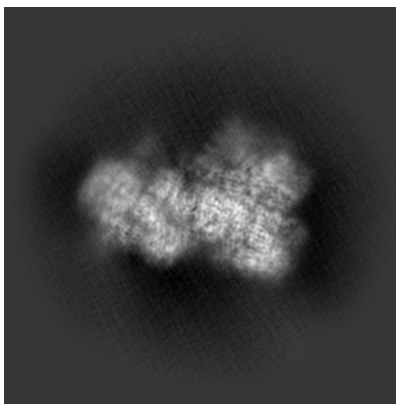
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

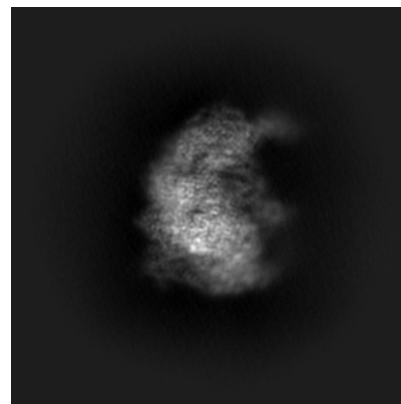
6.1.1 Primary map



X

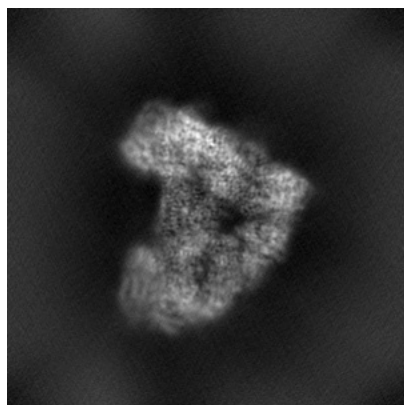


Y

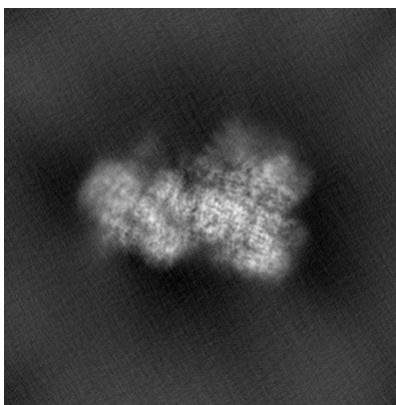


Z

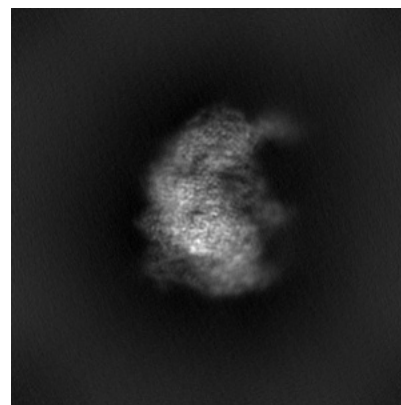
6.1.2 Raw map



X



Y

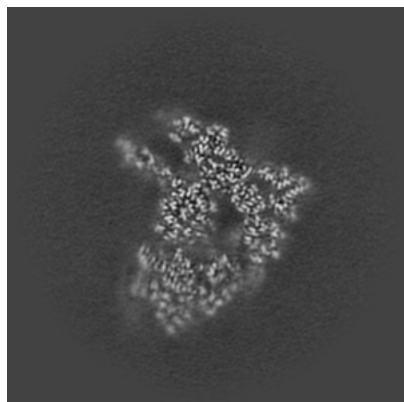


Z

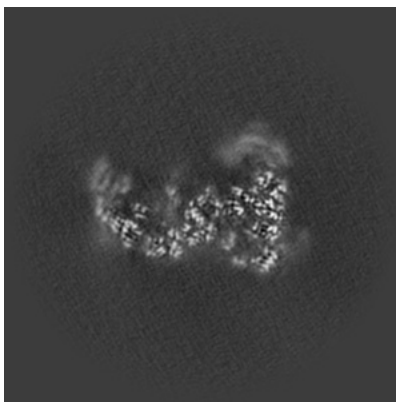
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

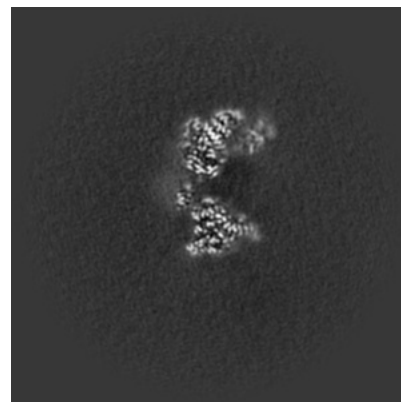
6.2.1 Primary map



X Index: 180

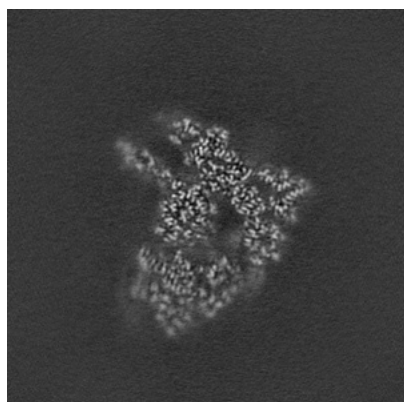


Y Index: 180

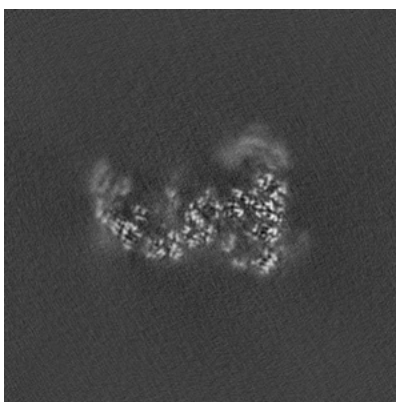


Z Index: 180

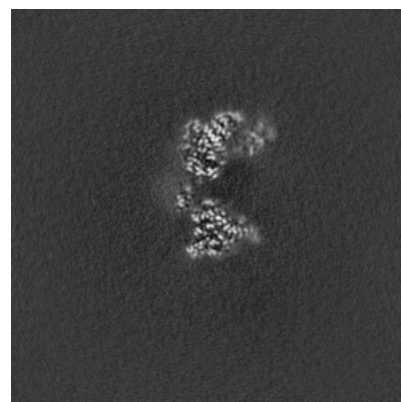
6.2.2 Raw map



X Index: 180



Y Index: 180

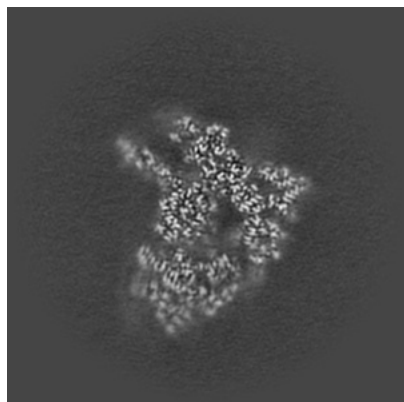


Z Index: 180

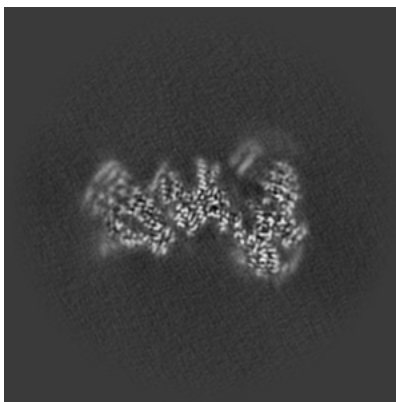
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

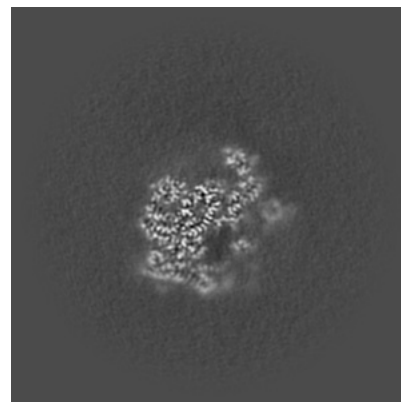
6.3.1 Primary map



X Index: 179

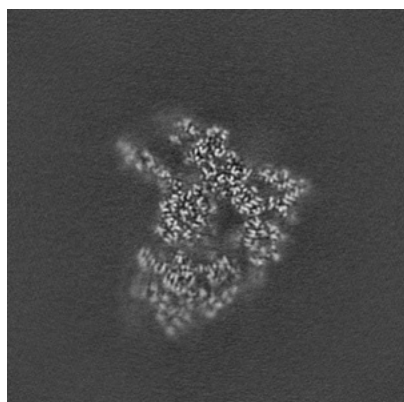


Y Index: 160

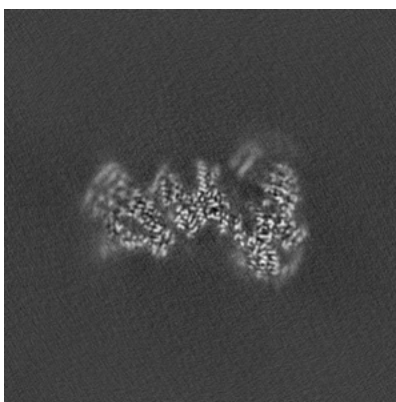


Z Index: 232

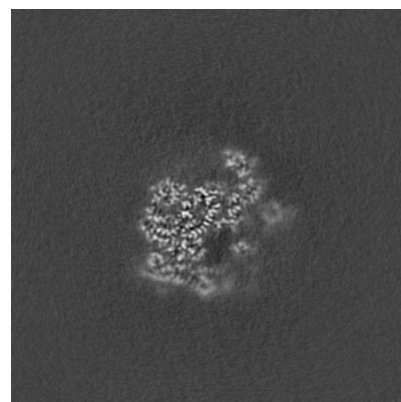
6.3.2 Raw map



X Index: 179



Y Index: 160

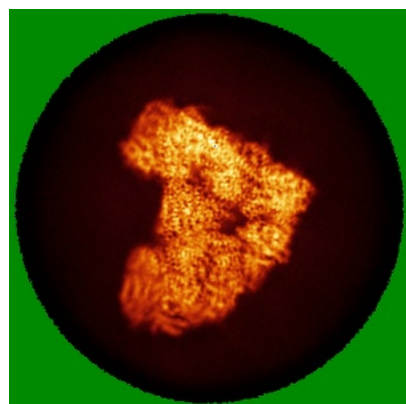


Z Index: 232

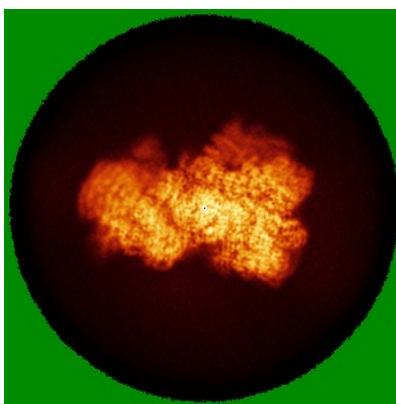
The images above show the largest variance slices of the map in three orthogonal directions.

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

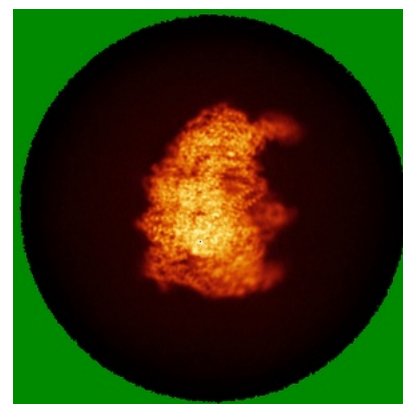
6.4.1 Primary map



X

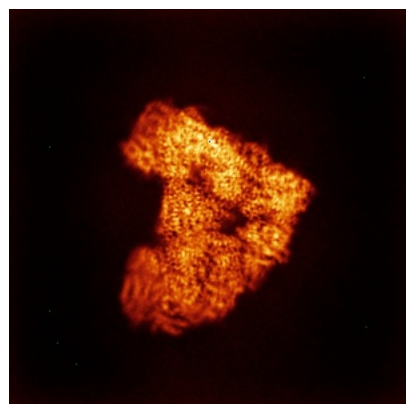


Y

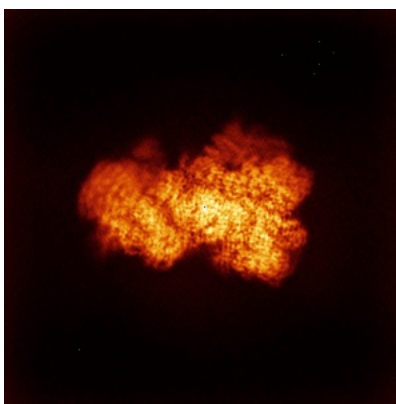


Z

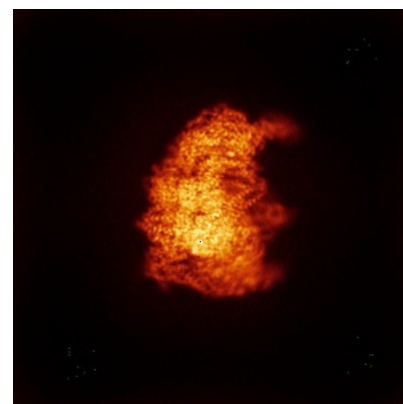
6.4.2 Raw map



X



Y

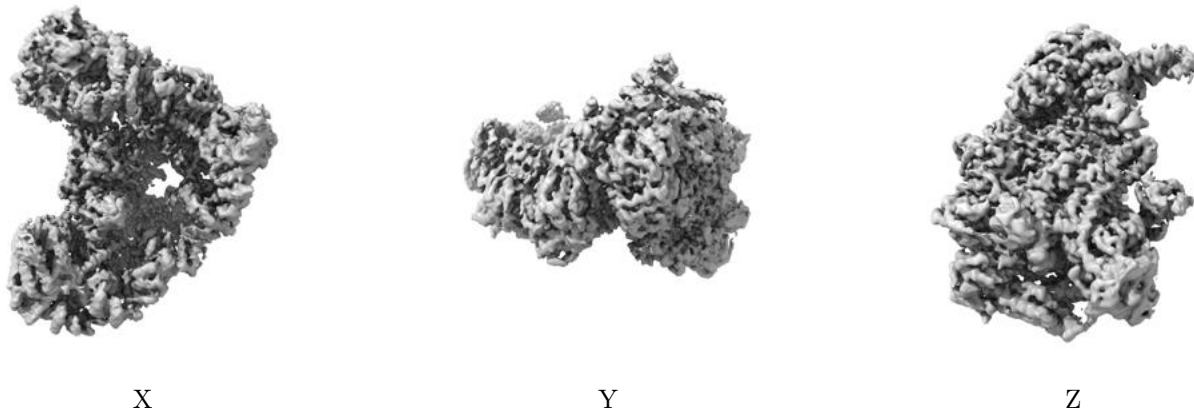


Z

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.

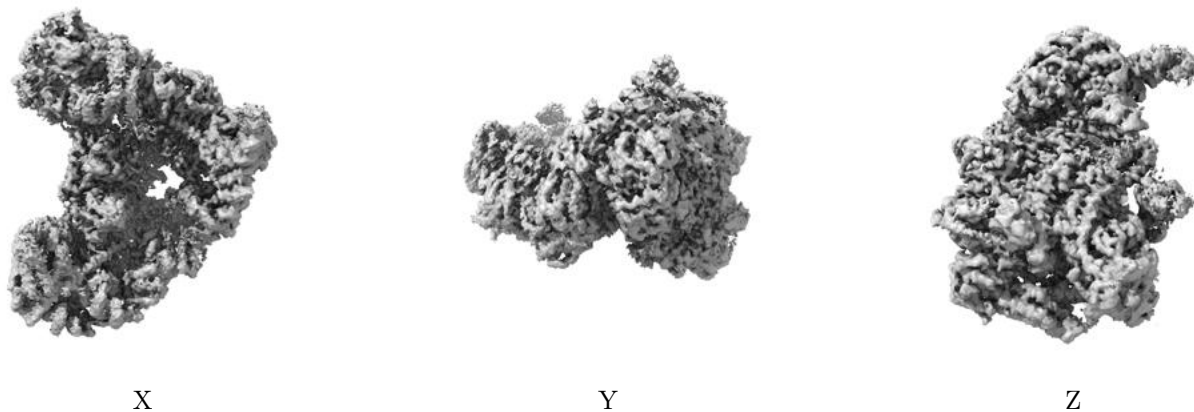
6.5 Orthogonal surface views [i](#)

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.

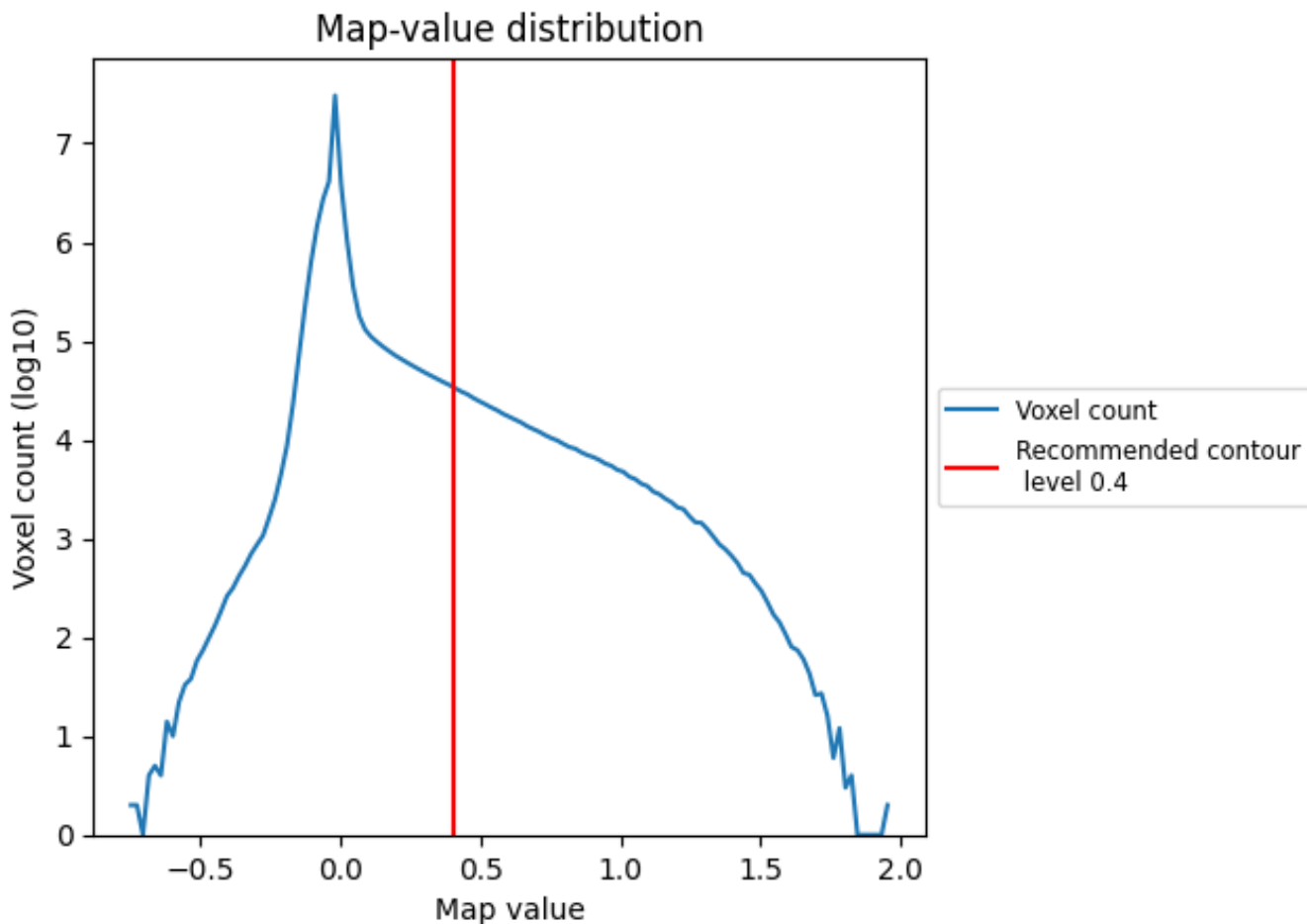
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

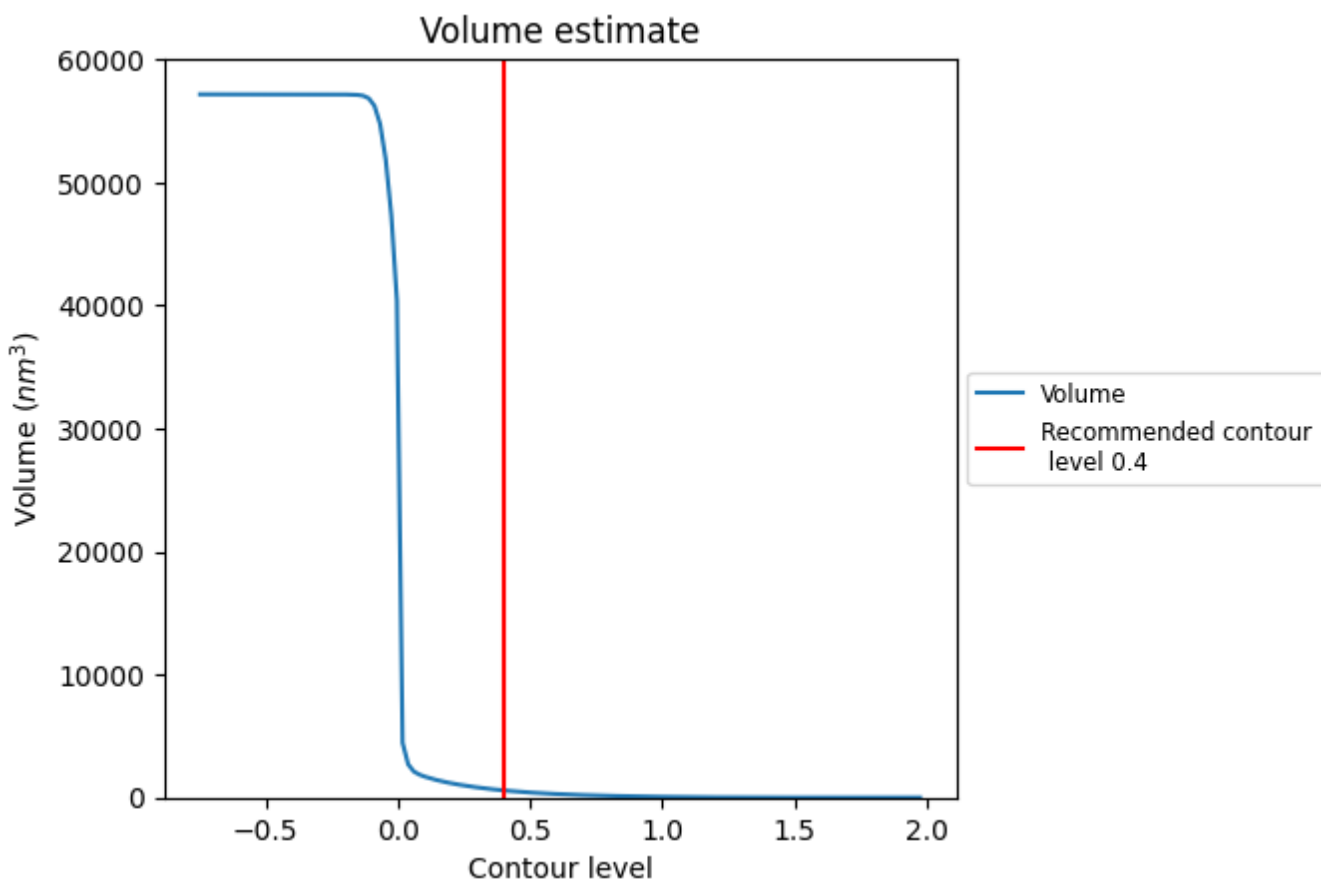
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

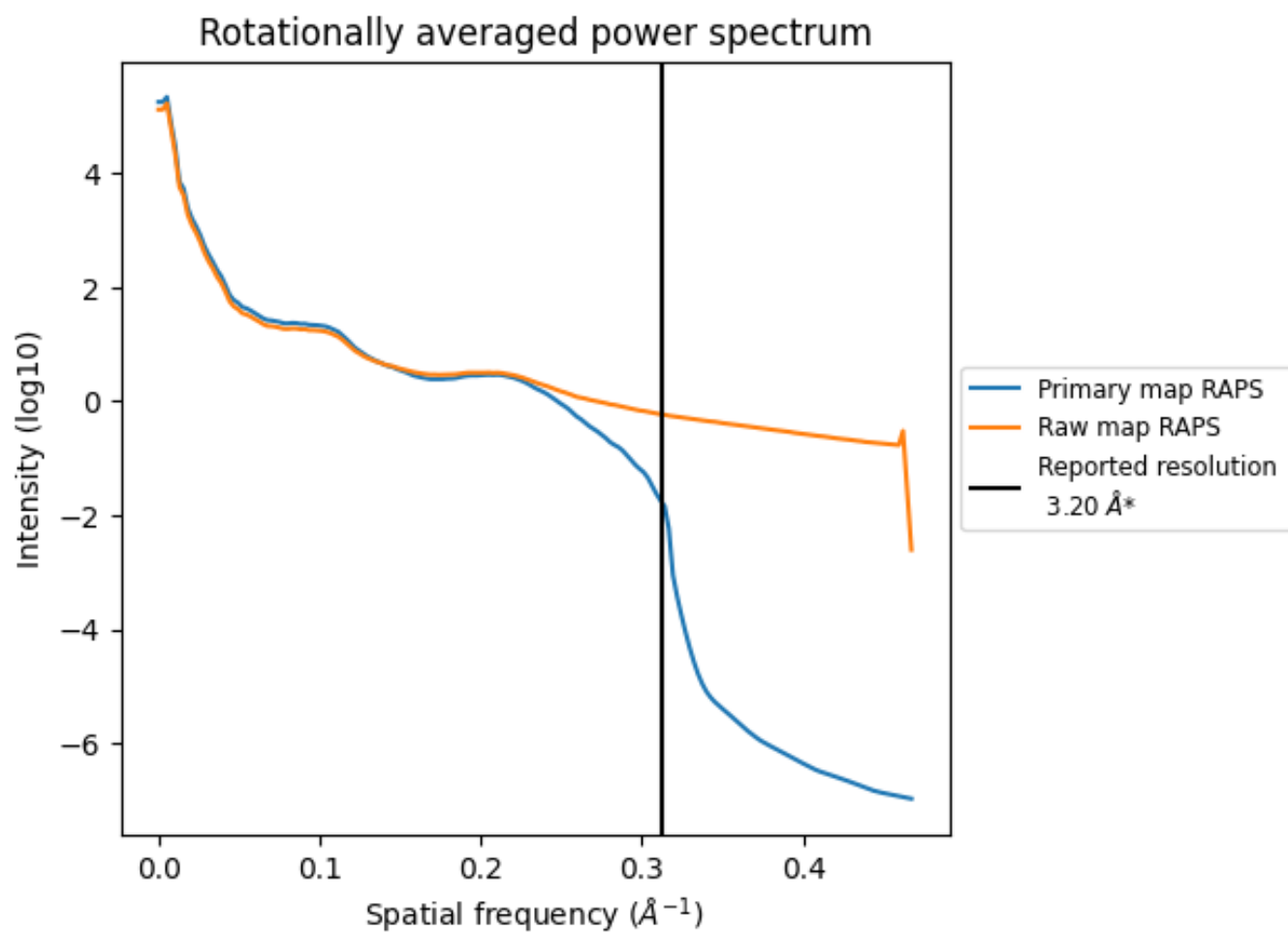
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 582 nm³; this corresponds to an approximate mass of 526 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

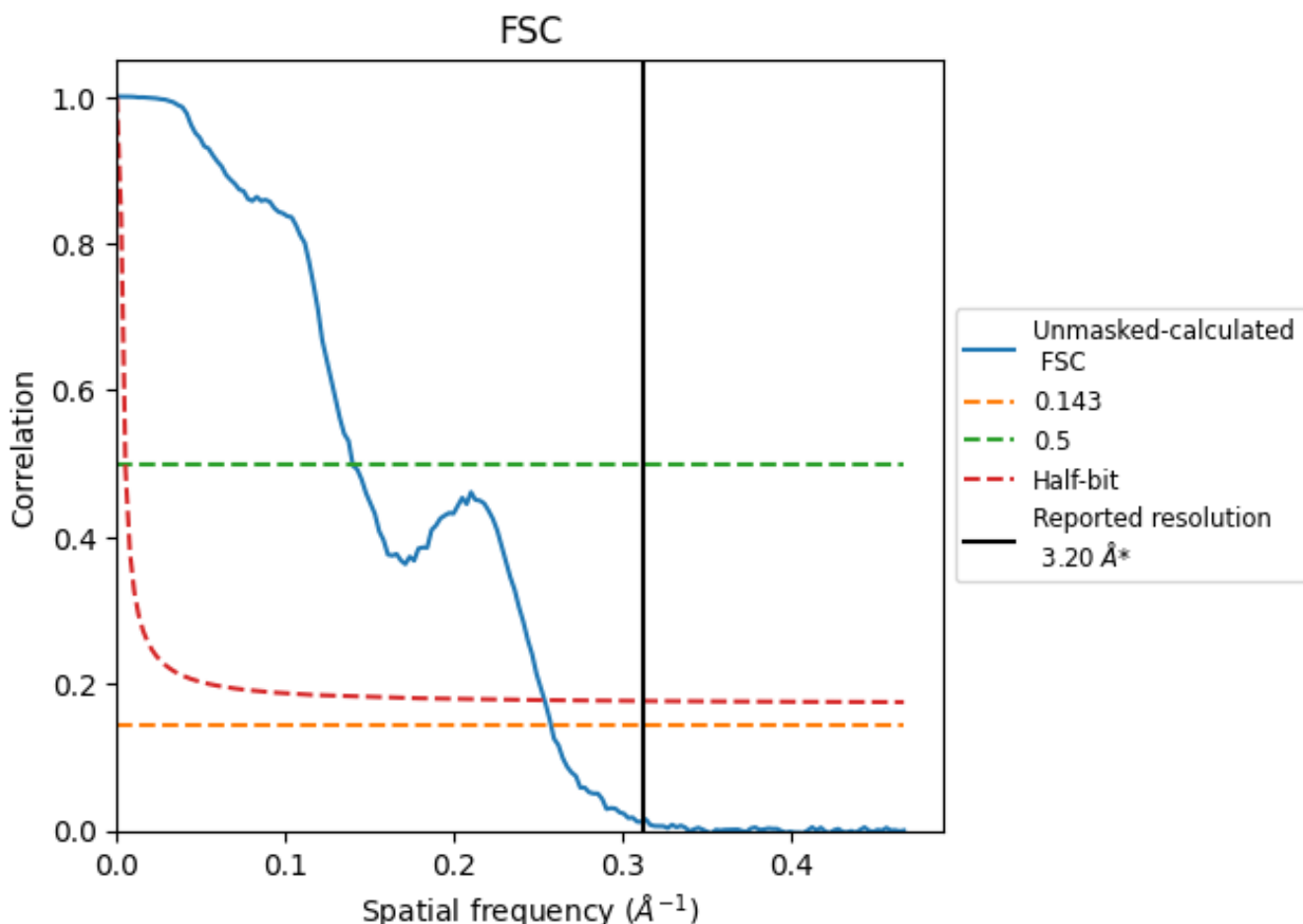


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

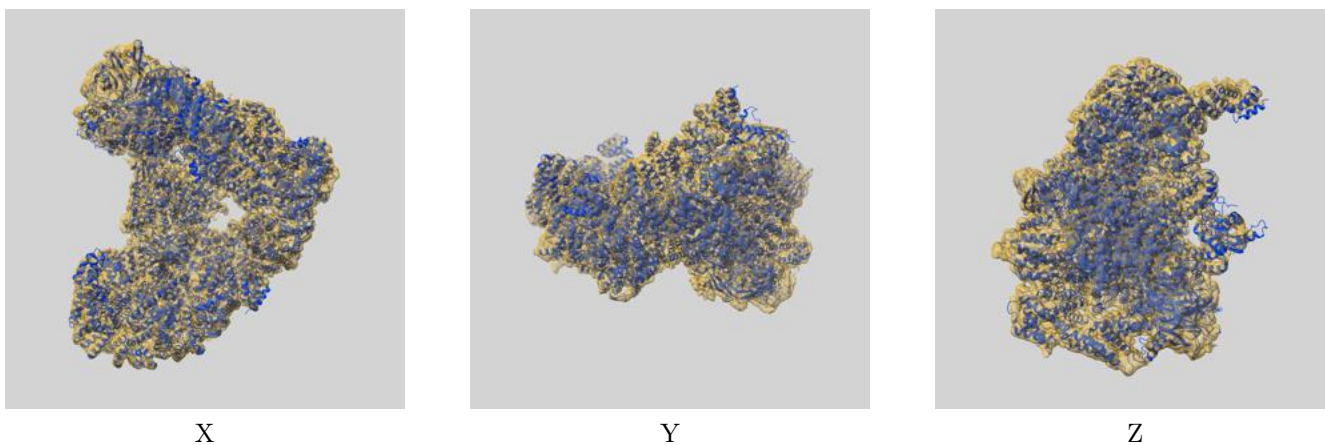
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	7.14	3.94

*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 3.88 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

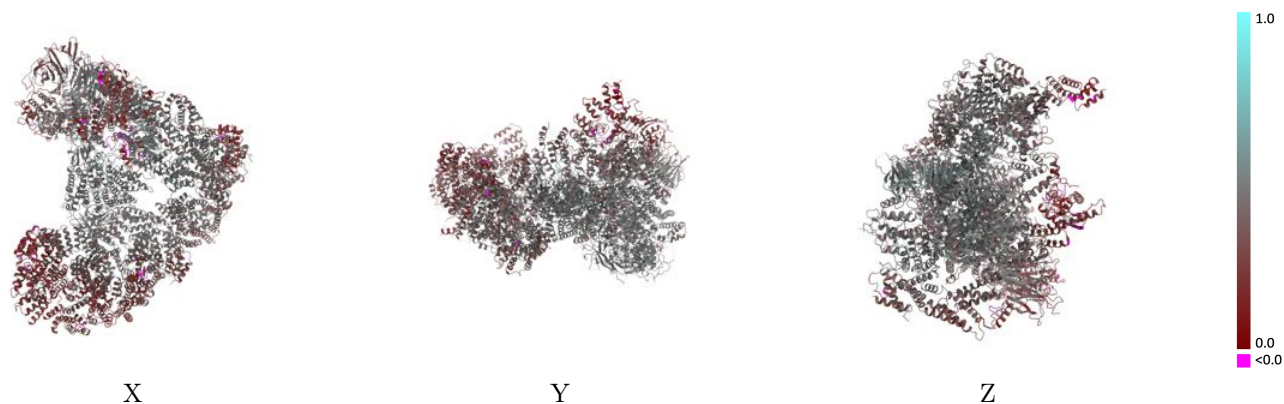
This section contains information regarding the fit between EMDB map EMD-17751 and PDB model 8PKP. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



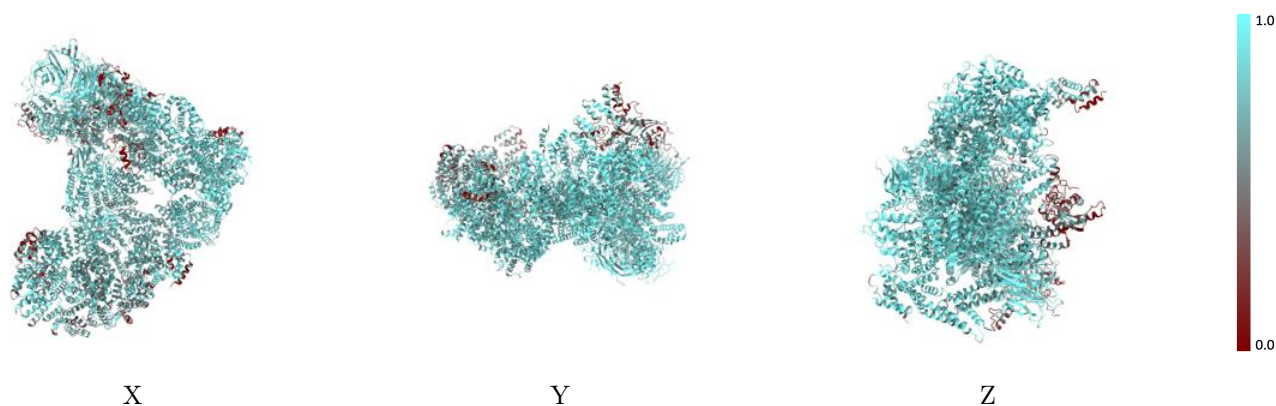
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



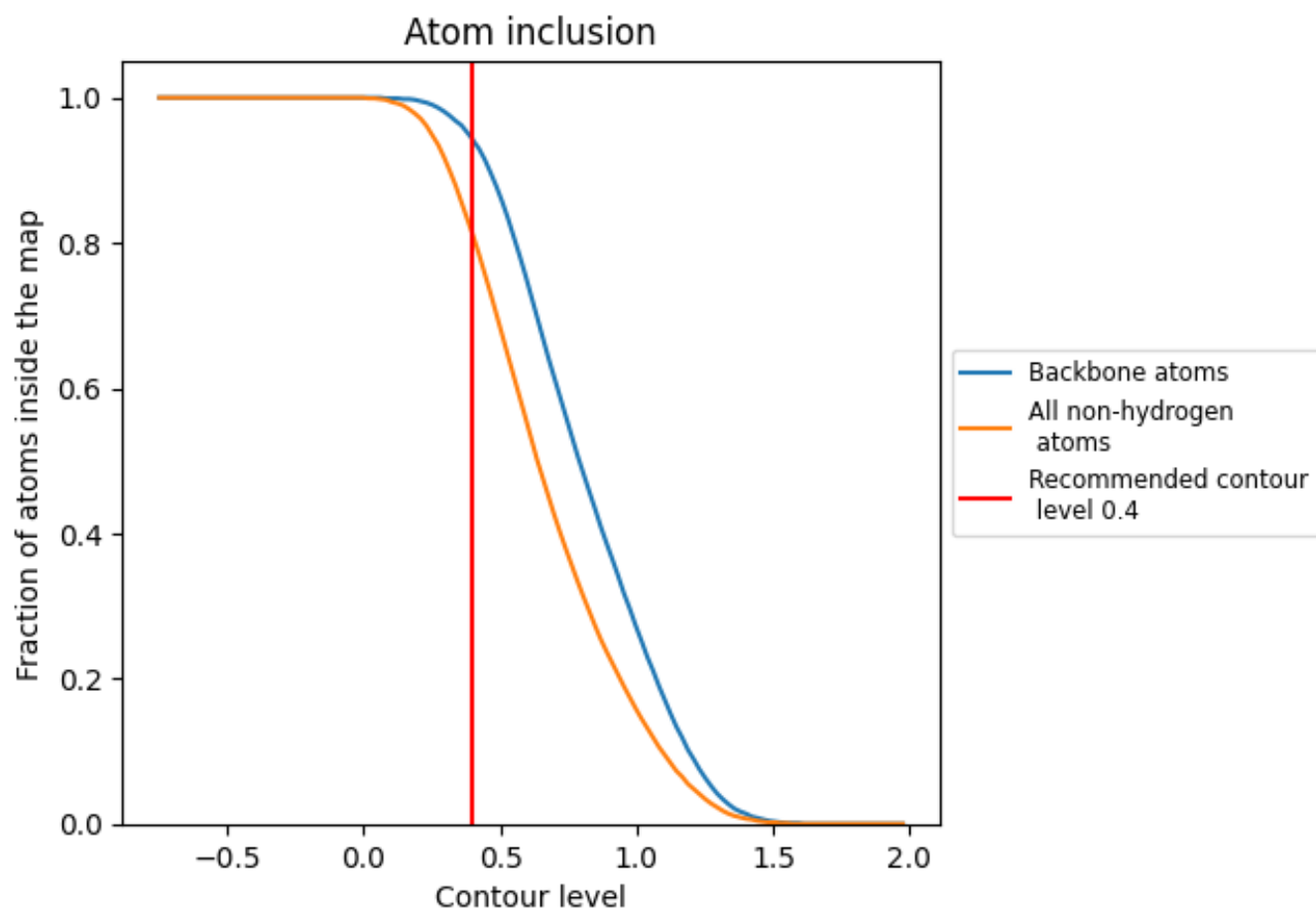
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 94% of all backbone atoms, 81% 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	 0.8100	 0.4090
A	 0.8920	 0.4780
C	 0.1070	 0.1150
D	 0.7850	 0.4620
G	 0.7840	 0.4230
H	 0.7700	 0.3860
I	 0.8390	 0.4210
J	 0.7830	 0.3820
K	 0.8580	 0.4400
L	 0.8310	 0.4350
M	 0.7420	 0.4490
N	 0.6350	 0.3290
O	 0.8860	 0.4750
P	 0.8590	 0.4300
Q	 0.8640	 0.4160
U	 0.8280	 0.4020
V	 0.8800	 0.4700
W	 0.7800	 0.4880
Y	 0.6700	 0.2650
Z	 0.6850	 0.2580

