



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:43 AM UTC

PDB ID : 8A61 / pdb_00008a61
EMDB ID : EMD-15201
Title : S. cerevisiae apo phosphorylated APC/C
Authors : Barford, D.; Fernandez-Vazquez, E.; Zhang, Z.; Yang, J.
Deposited on : 2022-06-16
Resolution : 5.40 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:

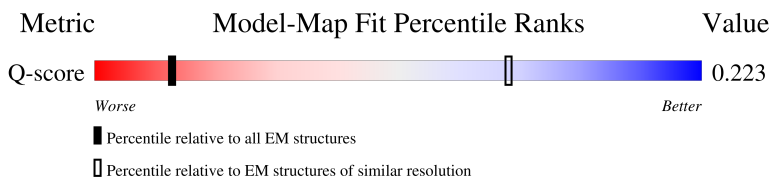
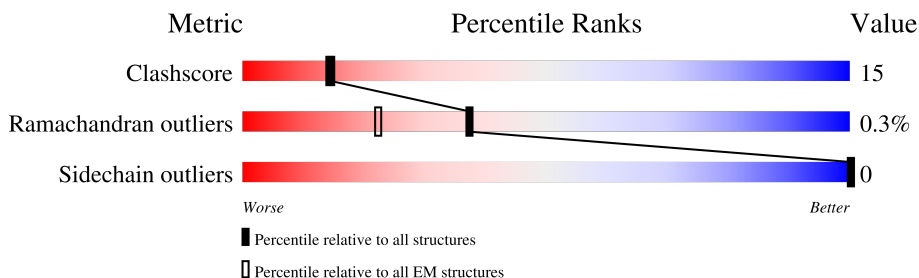
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 5.40 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.




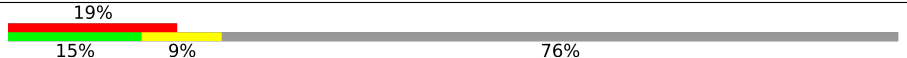
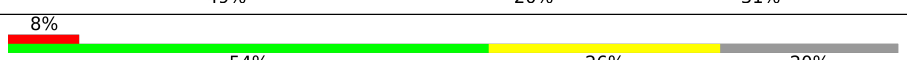

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	538 (4.90 - 5.90)

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	F	758	<p>43% 23% 34%</p>
1	H	758	<p>16% 44% 23% 33%</p>
2	J	850	<p>38% 22% 40%</p>
2	K	850	<p>13% 39% 21% 41%</p>

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Mol	Chain	Length	Quality of chain
3	G	124	 14% 14% 73%
3	W	124	 19% 15% 9% 76%
4	E	265	 21% 37% 12% 51%
5	T	853	 17% 56% 20% 24%
6	U	165	 39% 49% 20% 31%
7	C	1748	 8% 54% 26% 20%
8	O	685	 64% 32% 6% .
9	D	626	 6% 60% 30% 11%
9	P	626	 61% 27% 11% .
10	I	170	 9% 36% 26% 37%
11	N	368	 16% 10% 74%
12	Q	652	 7% 67% 29% .
13	A	250	 23% 52% 35% 13%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 57784 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 CDC27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	502	3991	2569	656	739	27	0	0
1	H	505	4038	2599	664	748	27	0	0

- Molecule 2 is a protein called Anaphase-promoting complex subunit CDC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	509	4124	2658	674	769	23	0	0
2	K	505	4102	2642	673	764	23	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	841	LYS	-	expression tag	UNP P09798
J	842	SER	-	expression tag	UNP P09798
J	843	SER	-	expression tag	UNP P09798
J	844	ILE	-	expression tag	UNP P09798
J	845	PRO	-	expression tag	UNP P09798
J	846	GLU	-	expression tag	UNP P09798
J	847	ASN	-	expression tag	UNP P09798
J	848	LEU	-	expression tag	UNP P09798
J	849	TYR	-	expression tag	UNP P09798
J	850	PHE	-	expression tag	UNP P09798
K	841	LYS	-	expression tag	UNP P09798
K	842	SER	-	expression tag	UNP P09798
K	843	SER	-	expression tag	UNP P09798
K	844	ILE	-	expression tag	UNP P09798
K	845	PRO	-	expression tag	UNP P09798
K	846	GLU	-	expression tag	UNP P09798
K	847	ASN	-	expression tag	UNP P09798

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Chain	Residue	Modelled	Actual	Comment	Reference
K	848	LEU	-	expression tag	UNP P09798
K	849	TYR	-	expression tag	UNP P09798
K	850	PHE	-	expression tag	UNP P09798

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	34	Total	C	N	O	S	0	0
			275	169	50	55	1		
3	W	30	Total	C	N	O	S	0	0
			242	148	44	49	1		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	130	Total	C	N	O	S	0	0
			1091	678	201	205	7		

- Molecule 5 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	T	650	Total	C	N	O	S	0	0
			5362	3476	877	985	24		

- Molecule 6 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	U	114	Total	C	N	O	S	0	0
			912	574	164	162	12		

- Molecule 7 is a protein called Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	1406	Total	C	N	O	S	0	0
			10832	7003	1749	2034	46		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	658	Total	C	N	O	S	0	0
			5285	3399	869	990	27		

- Molecule 9 is a protein called Anaphase-promoting complex subunit CDC23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	560	Total	C	N	O	S	0	0
			4524	2925	729	844	26		
9	P	556	Total	C	N	O	S	0	0
			4520	2923	738	832	27		

- Molecule 10 is a protein called Anaphase-promoting complex subunit SWM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	107	Total	C	N	O	S	0	0
			878	551	154	171	2		

- Molecule 11 is a protein called Anaphase-promoting complex subunit MND2.

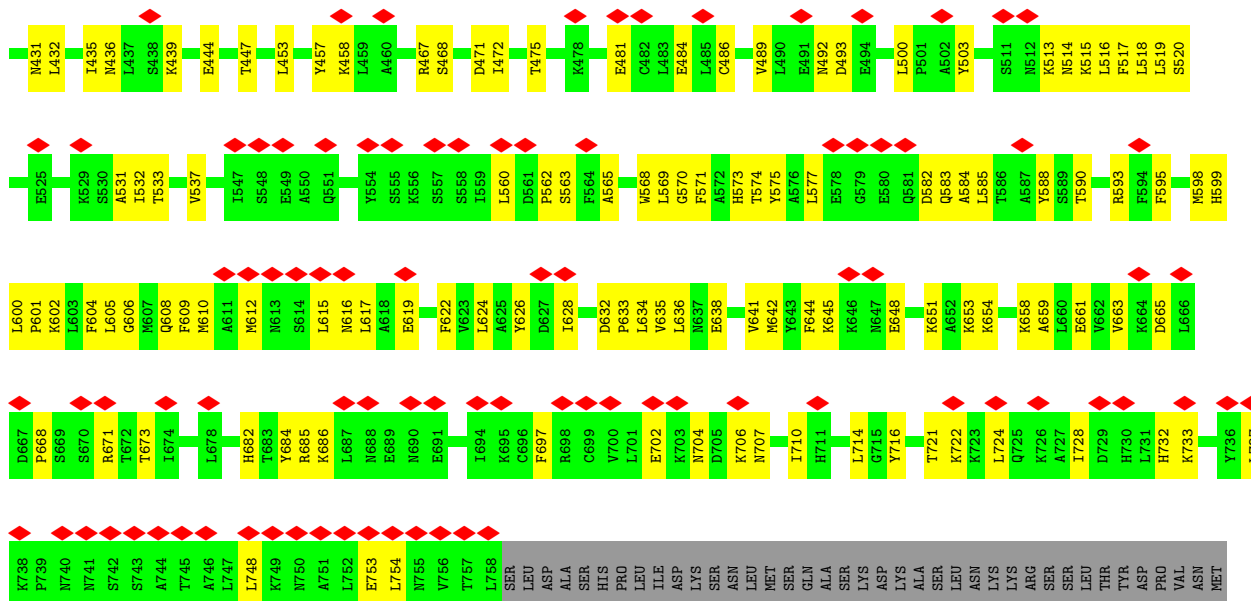
Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	96	Total	C	N	O	S	0	0
			784	504	138	139	3		

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

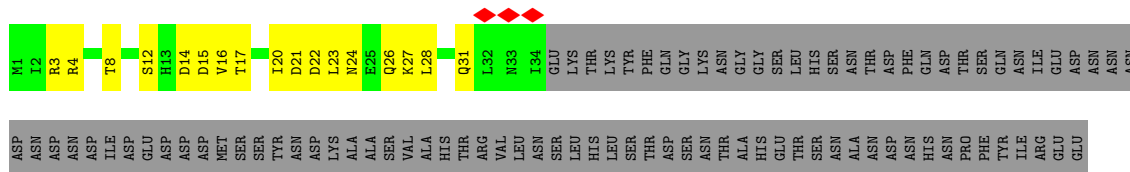
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	623	Total	C	N	O	S	0	0
			5086	3279	842	952	13		

- Molecule 13 is a protein called Anaphase-promoting complex subunit DOC1.

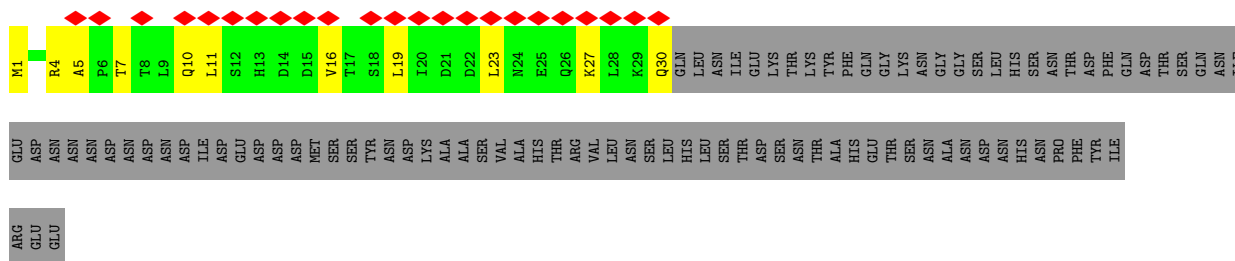
Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	218	Total	C	N	O	S	0	0
			1738	1113	303	312	10		



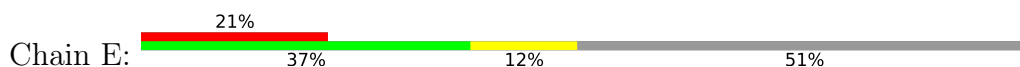
• Molecule 3: Anaphase-promoting complex subunit CDC26

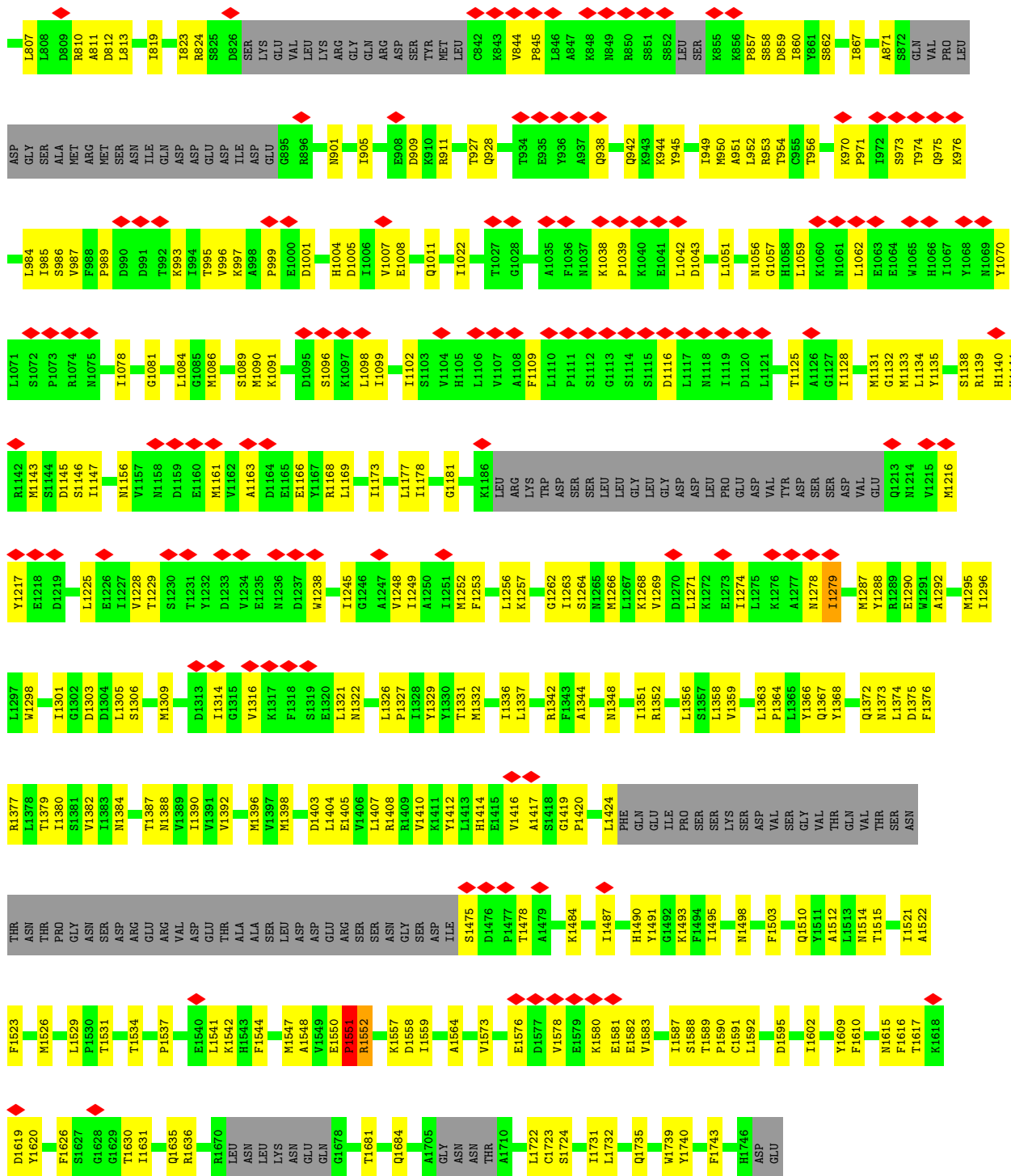


• Molecule 3: Anaphase-promoting complex subunit CDC26

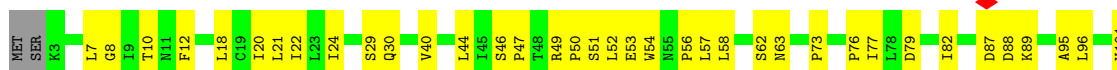


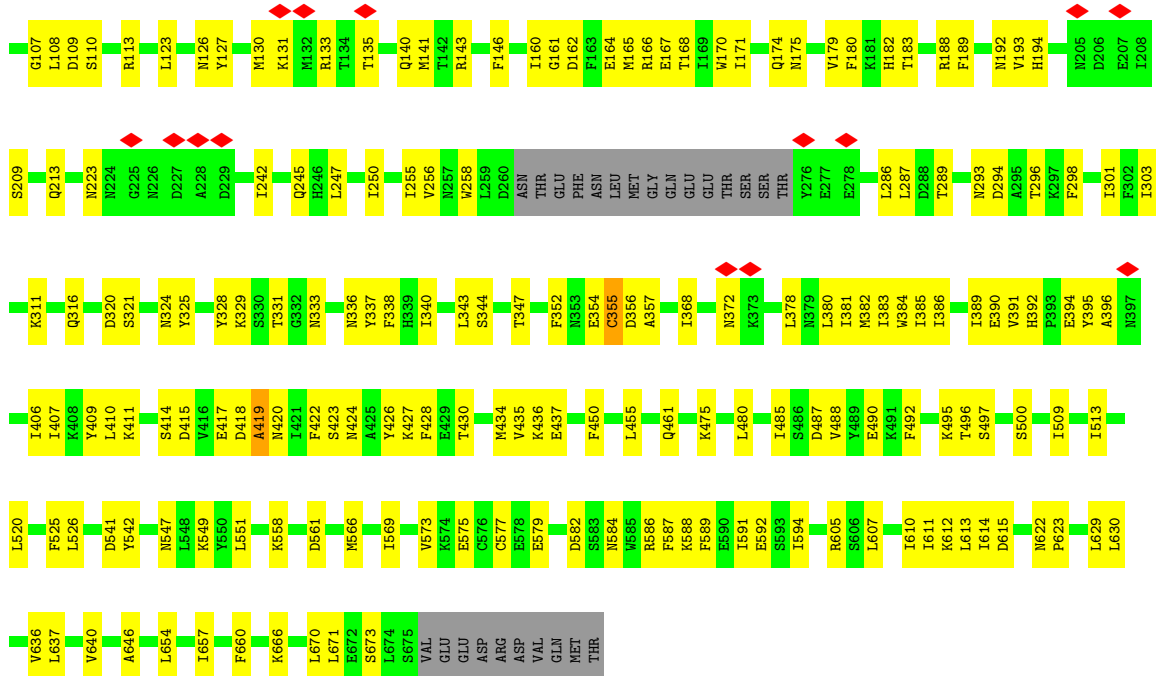
• Molecule 4: Anaphase-promoting complex subunit 9



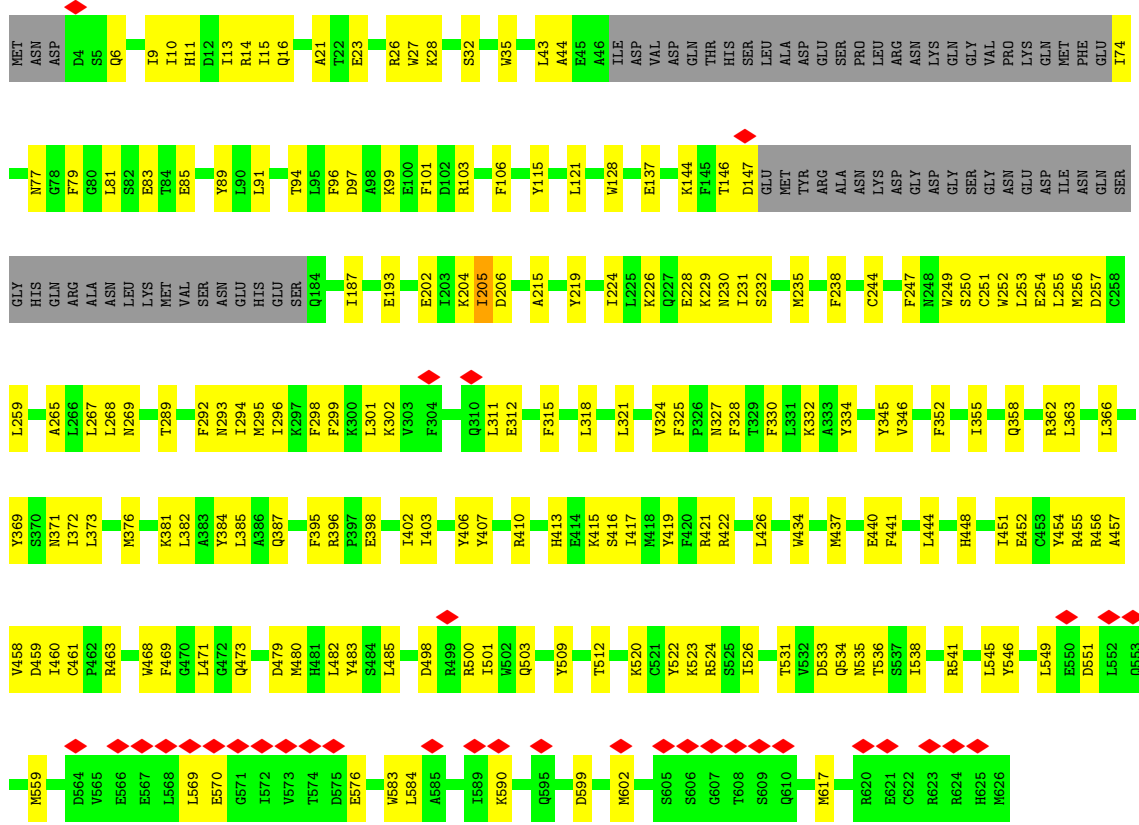


• Molecule 8: Anaphase-promoting complex subunit 5

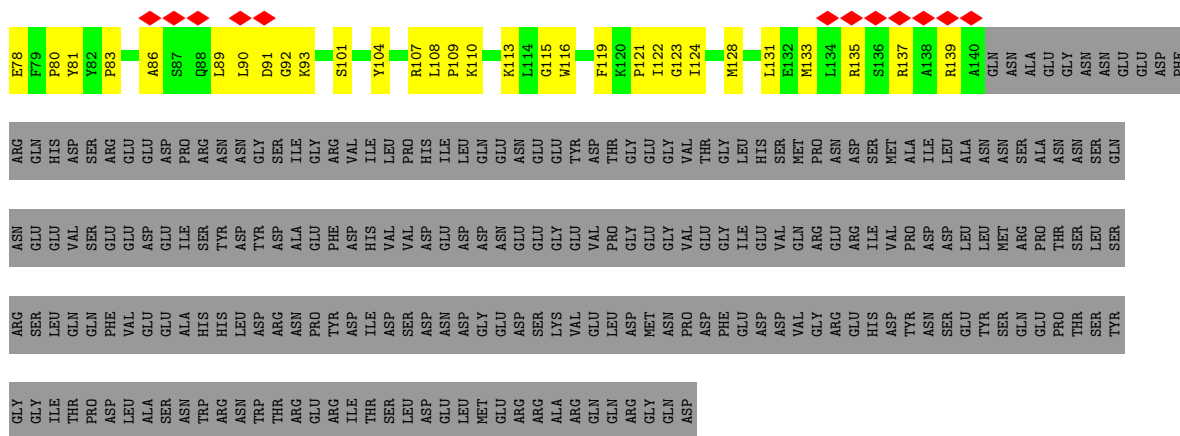




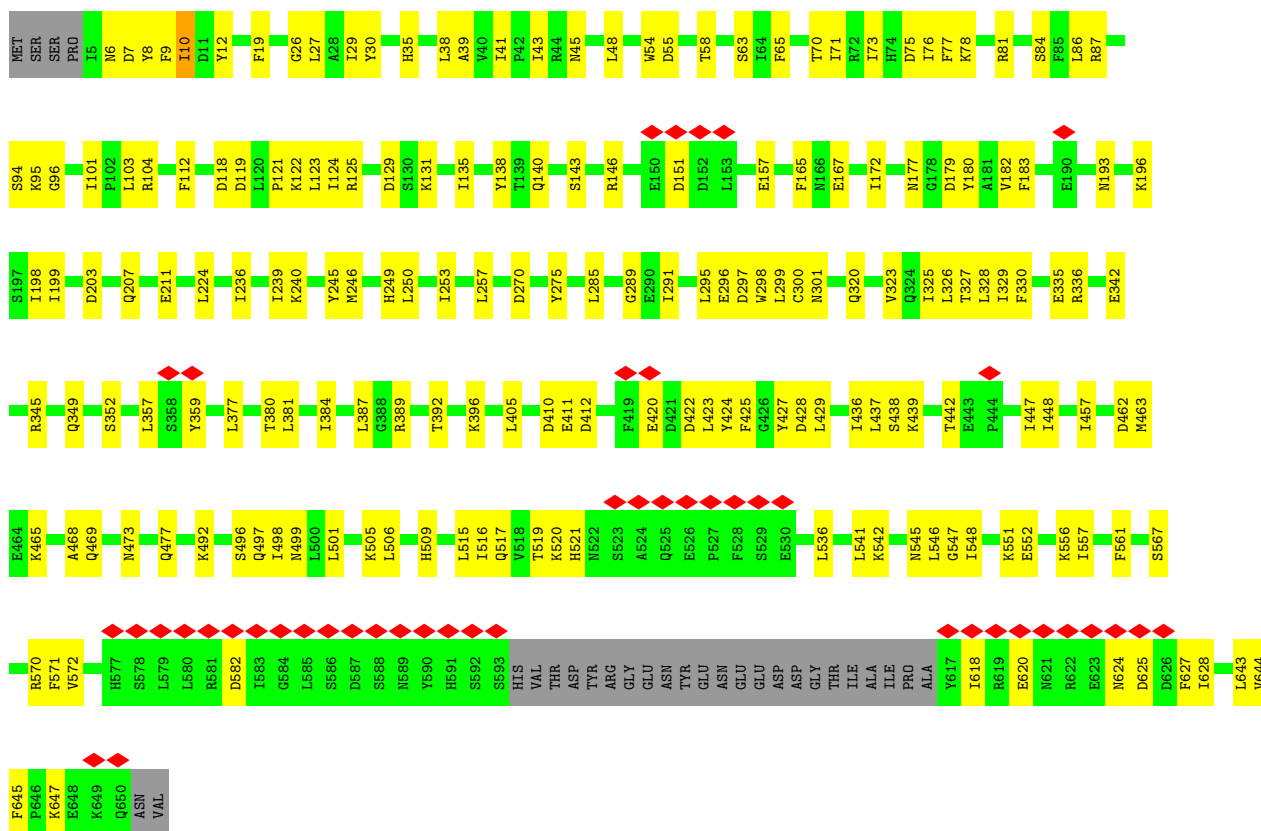
● Molecule 9: Anaphase-promoting complex subunit CDC23



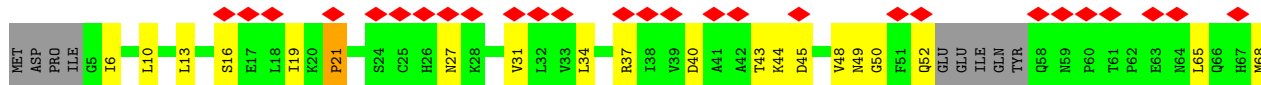
● Molecule 9: Anaphase-promoting complex subunit CDC23

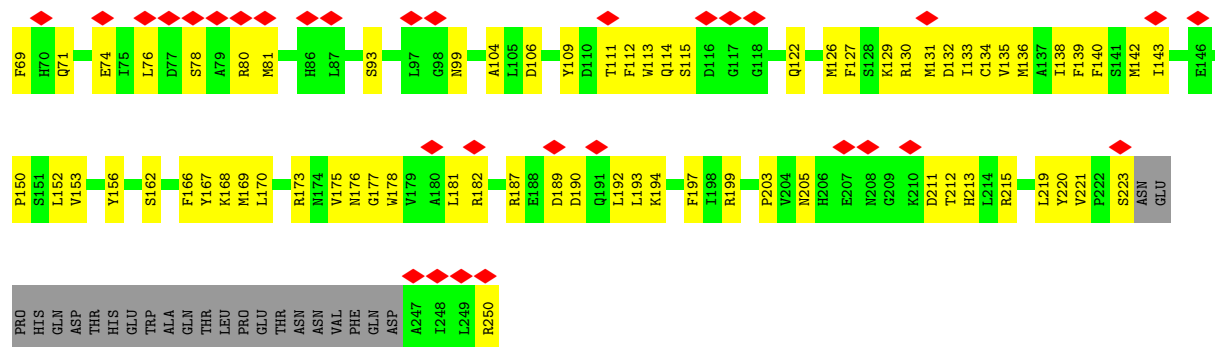


• Molecule 12: Anaphase-promoting complex subunit 4



• Molecule 13: Anaphase-promoting complex subunit DOC1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	2600	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	F	0.15	0/4079	0.38	0/5525
1	H	0.15	0/4126	0.35	0/5585
2	J	0.20	0/4210	0.42	0/5688
2	K	0.16	0/4188	0.40	1/5657 (0.0%)
3	G	0.19	0/276	0.57	0/372
3	W	0.20	0/243	0.44	0/327
4	E	0.12	0/1108	0.31	0/1481
5	T	0.13	0/5479	0.32	0/7420
6	U	0.12	0/936	0.30	0/1265
7	C	0.16	0/11057	0.35	1/15038 (0.0%)
8	O	0.20	0/5384	0.35	0/7287
9	D	0.18	0/4621	0.36	0/6243
9	P	0.17	0/4618	0.33	0/6231
10	I	0.22	0/902	0.43	0/1226
11	N	0.16	0/800	0.39	0/1076
12	Q	0.16	0/5193	0.32	0/7024
13	A	0.15	0/1780	0.38	0/2411
All	All	0.17	0/59000	0.36	2/79856 (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
5	T	0	2
7	C	0	1
10	I	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	845	PRO	N-CA-CB	6.67	110.26	103.25
2	K	357	MET	CB-CG-SD	-5.13	97.32	112.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	1551	PRO	Peptide
10	I	35	PRO	Peptide
5	T	620	THR	Peptide
5	T	623	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3991	0	3947	133	0
1	H	4038	0	4010	148	0
2	J	4124	0	4085	160	0
2	K	4102	0	4065	139	0
3	G	275	0	287	20	0
3	W	242	0	251	15	0
4	E	1091	0	1058	26	0
5	T	5362	0	5336	122	0
6	U	912	0	882	34	0
7	C	10832	0	10637	351	0
8	O	5285	0	5290	178	0
9	D	4524	0	4391	160	0
9	P	4520	0	4415	141	0
10	I	878	0	783	57	0
11	N	784	0	784	31	0
12	Q	5086	0	5095	138	0
13	A	1738	0	1705	86	0
All	All	57784	0	57021	1751	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 15.

The worst 5 of 1751 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:K:307:VAL:HG22	2:K:368:ILE:HD11	1.51	0.91
5:T:578:ASP:HB2	6:U:56:LYS:HZ1	1.36	0.91
9:P:247:PHE:HA	9:P:295:MET:HE1	1.53	0.90
5:T:225:CYS:HB3	5:T:229:MET:HE2	1.52	0.89
7:C:1131:MET:HE1	7:C:1147:ILE:HD11	1.54	0.88

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	F	496/758 (65%)	477 (96%)	19 (4%)	0	100	100
1	H	499/758 (66%)	484 (97%)	13 (3%)	2 (0%)	30	67
2	J	505/850 (59%)	481 (95%)	24 (5%)	0	100	100
2	K	501/850 (59%)	491 (98%)	10 (2%)	0	100	100
3	G	32/124 (26%)	32 (100%)	0	0	100	100
3	W	28/124 (23%)	28 (100%)	0	0	100	100
4	E	120/265 (45%)	118 (98%)	2 (2%)	0	100	100
5	T	638/853 (75%)	619 (97%)	17 (3%)	2 (0%)	36	71
6	U	110/165 (67%)	108 (98%)	2 (2%)	0	100	100
7	C	1380/1748 (79%)	1289 (93%)	85 (6%)	6 (0%)	30	67
8	O	654/685 (96%)	619 (95%)	31 (5%)	4 (1%)	21	59
9	D	554/626 (88%)	533 (96%)	20 (4%)	1 (0%)	43	77
9	P	550/626 (88%)	527 (96%)	22 (4%)	1 (0%)	43	77
10	I	101/170 (59%)	94 (93%)	7 (7%)	0	100	100
11	N	92/368 (25%)	86 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Q	619/652 (95%)	596 (96%)	22 (4%)	1 (0%)	43	77
13	A	212/250 (85%)	204 (96%)	7 (3%)	1 (0%)	24	63
All	All	7091/9872 (72%)	6786 (96%)	287 (4%)	18 (0%)	37	71

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	T	621	GLN
5	T	624	ASN
7	C	844	VAL
7	C	1279	ILE
7	C	1552	ARG

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	F	433/684 (63%)	433 (100%)	0	100	100
1	H	440/684 (64%)	440 (100%)	0	100	100
2	J	450/760 (59%)	450 (100%)	0	100	100
2	K	448/760 (59%)	448 (100%)	0	100	100
3	G	33/115 (29%)	33 (100%)	0	100	100
3	W	29/115 (25%)	29 (100%)	0	100	100
4	E	123/246 (50%)	123 (100%)	0	100	100
5	T	608/804 (76%)	608 (100%)	0	100	100
6	U	103/149 (69%)	103 (100%)	0	100	100
7	C	1177/1568 (75%)	1177 (100%)	0	100	100
8	O	597/643 (93%)	597 (100%)	0	100	100
9	D	477/560 (85%)	477 (100%)	0	100	100
9	P	477/560 (85%)	477 (100%)	0	100	100
10	I	92/144 (64%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	N	83/332 (25%)	83 (100%)	0	100	100
12	Q	572/598 (96%)	572 (100%)	0	100	100
13	A	190/226 (84%)	190 (100%)	0	100	100
All	All	6332/8948 (71%)	6332 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
9	P	287	GLN
9	P	514	ASN
12	Q	469	GLN
2	K	276	ASN
2	K	271	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

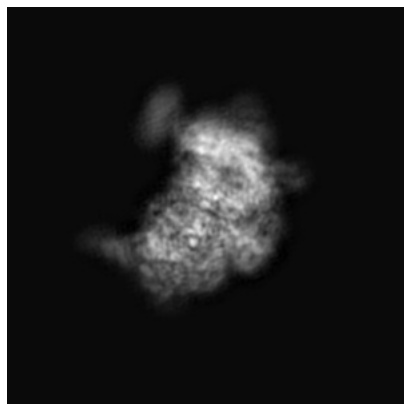
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15201. These allow visual inspection of the internal detail of the map and identification of artifacts.

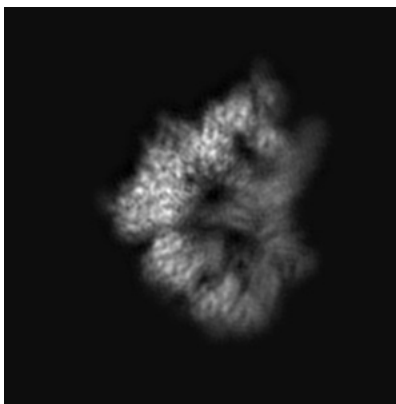
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

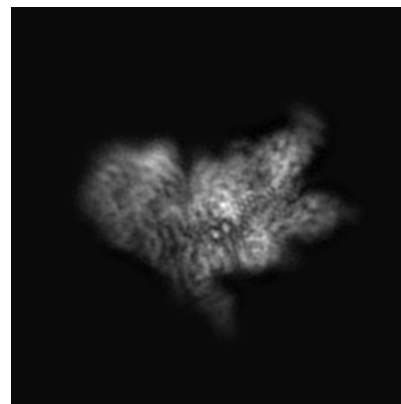
6.1.1 Primary map



X

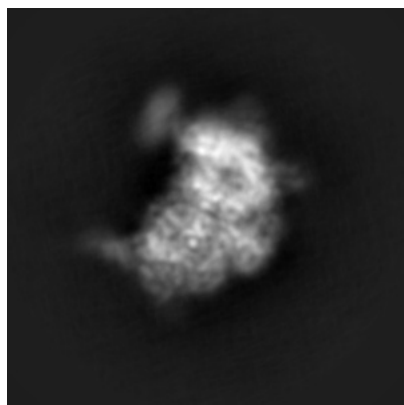


Y

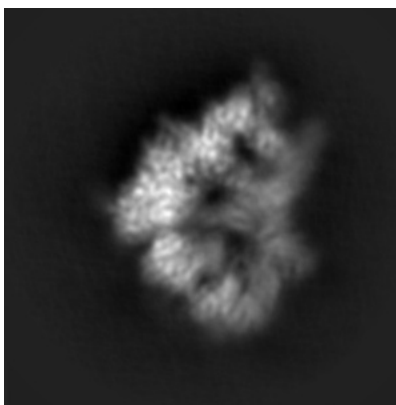


Z

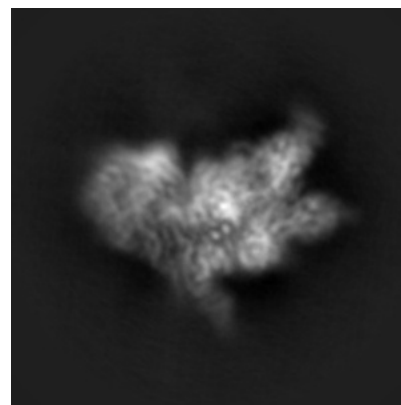
6.1.2 Raw map



X



Y

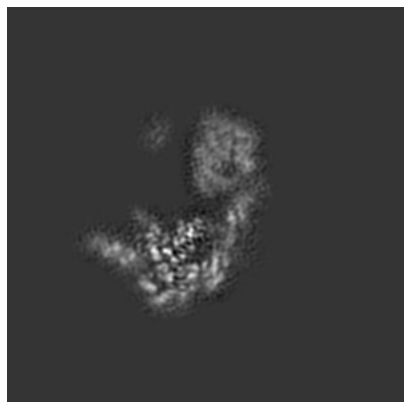


Z

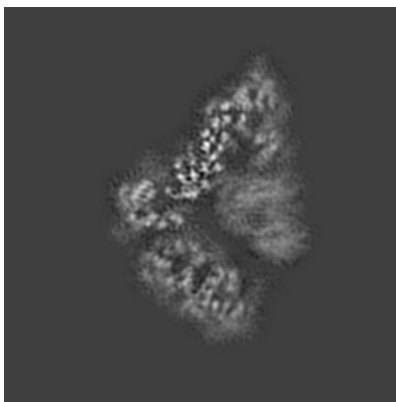
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

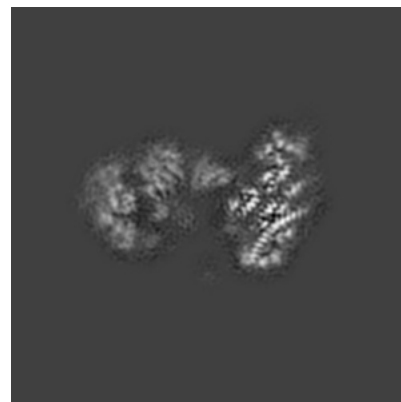
6.2.1 Primary map



X Index: 128

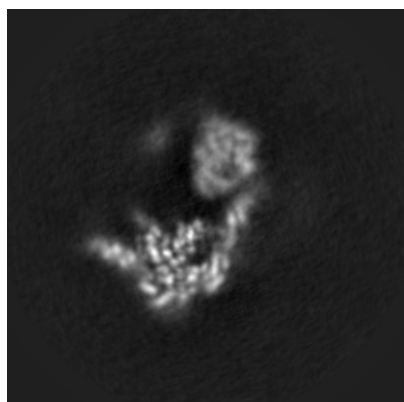


Y Index: 128

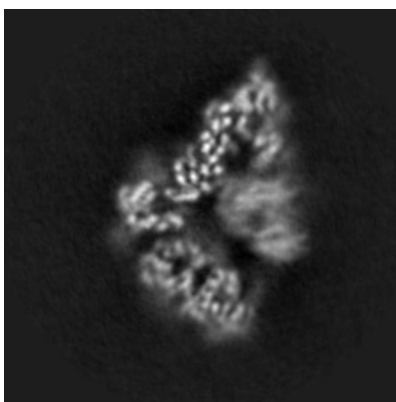


Z Index: 128

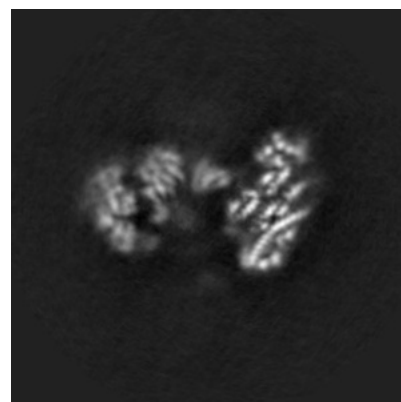
6.2.2 Raw map



X Index: 128



Y Index: 128

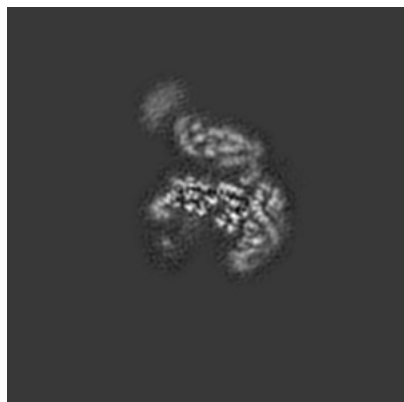


Z Index: 128

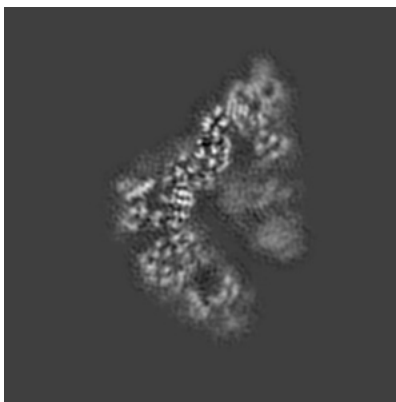
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

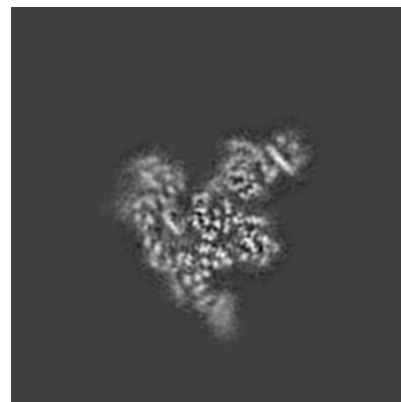
6.3.1 Primary map



X Index: 170

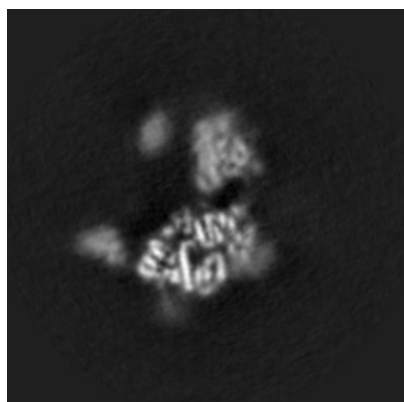


Y Index: 122

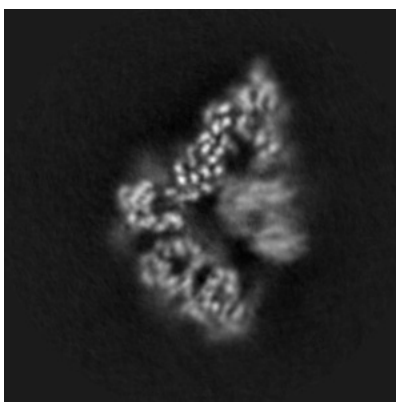


Z Index: 105

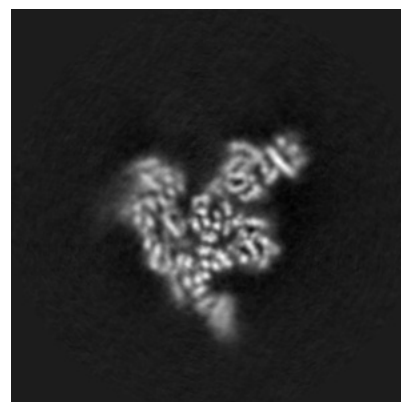
6.3.2 Raw map



X Index: 137



Y Index: 127

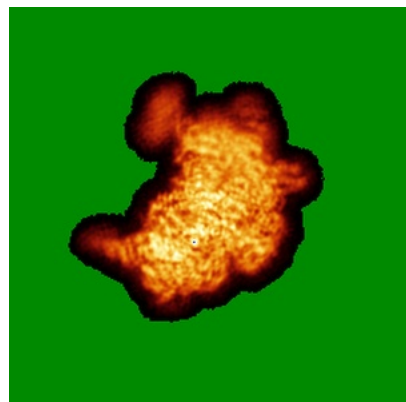


Z Index: 105

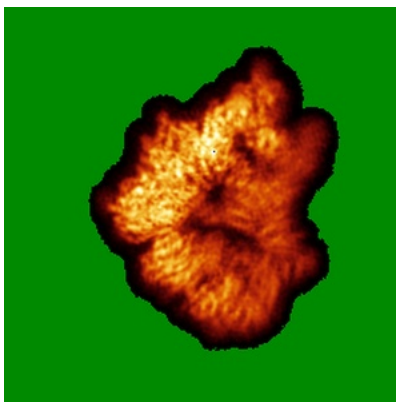
The images above show the largest variance slices of the map in three orthogonal directions.

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

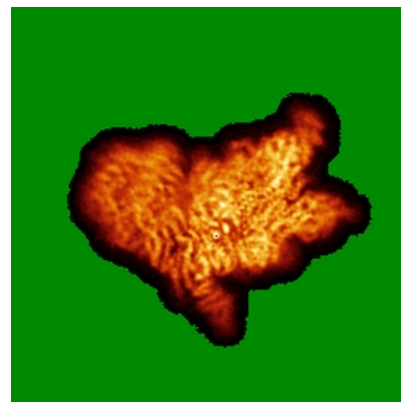
6.4.1 Primary map



X

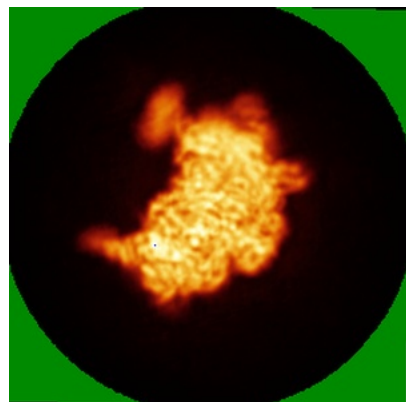


Y

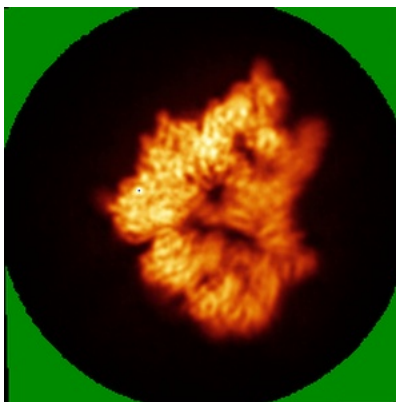


Z

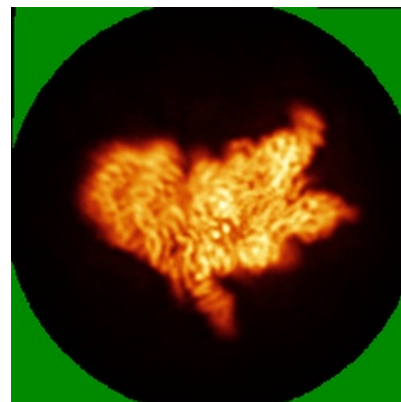
6.4.2 Raw map



X



Y



Z

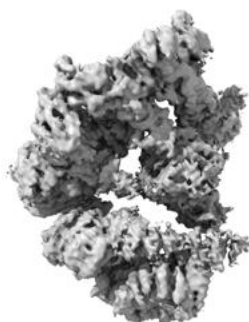
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

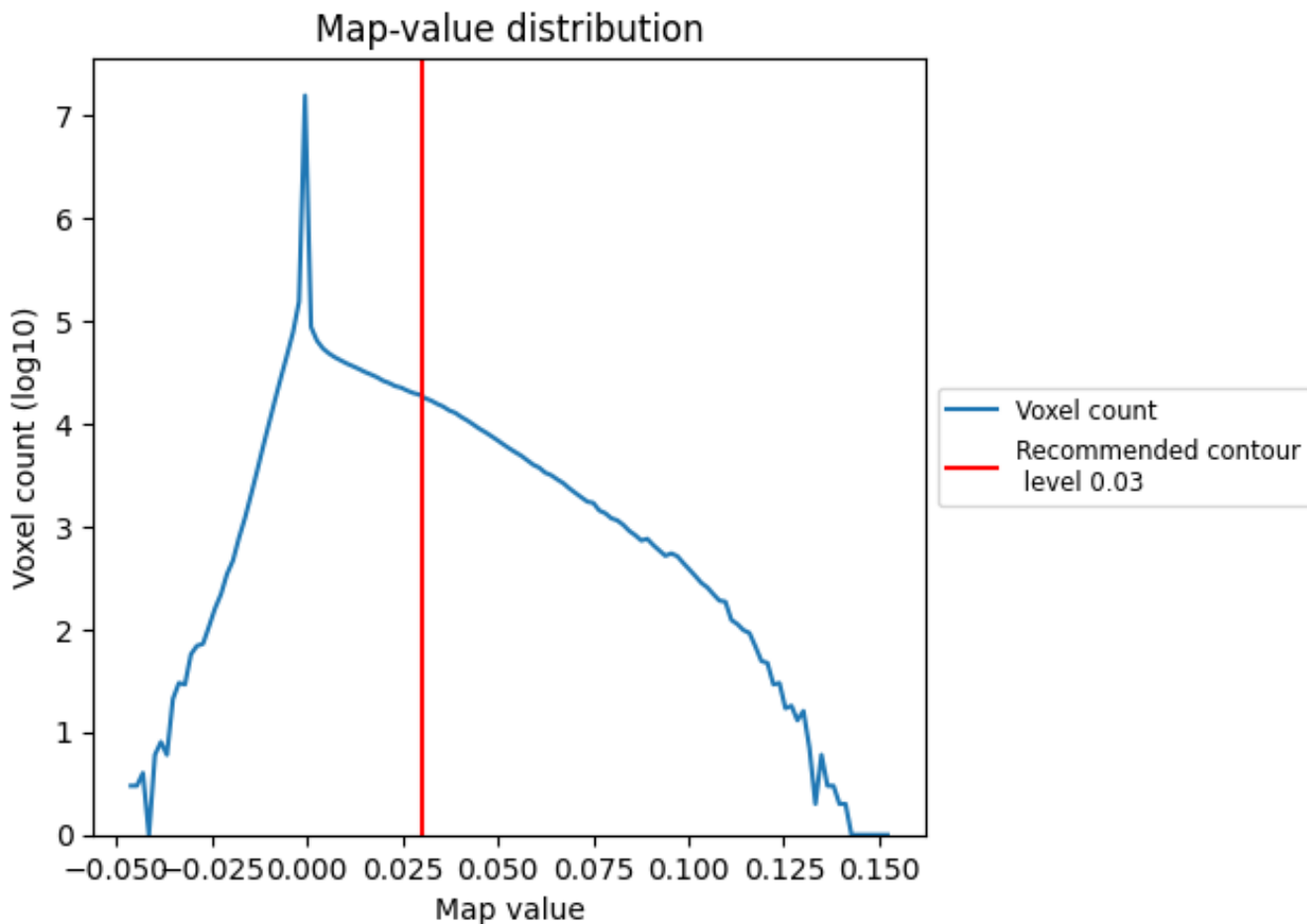
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

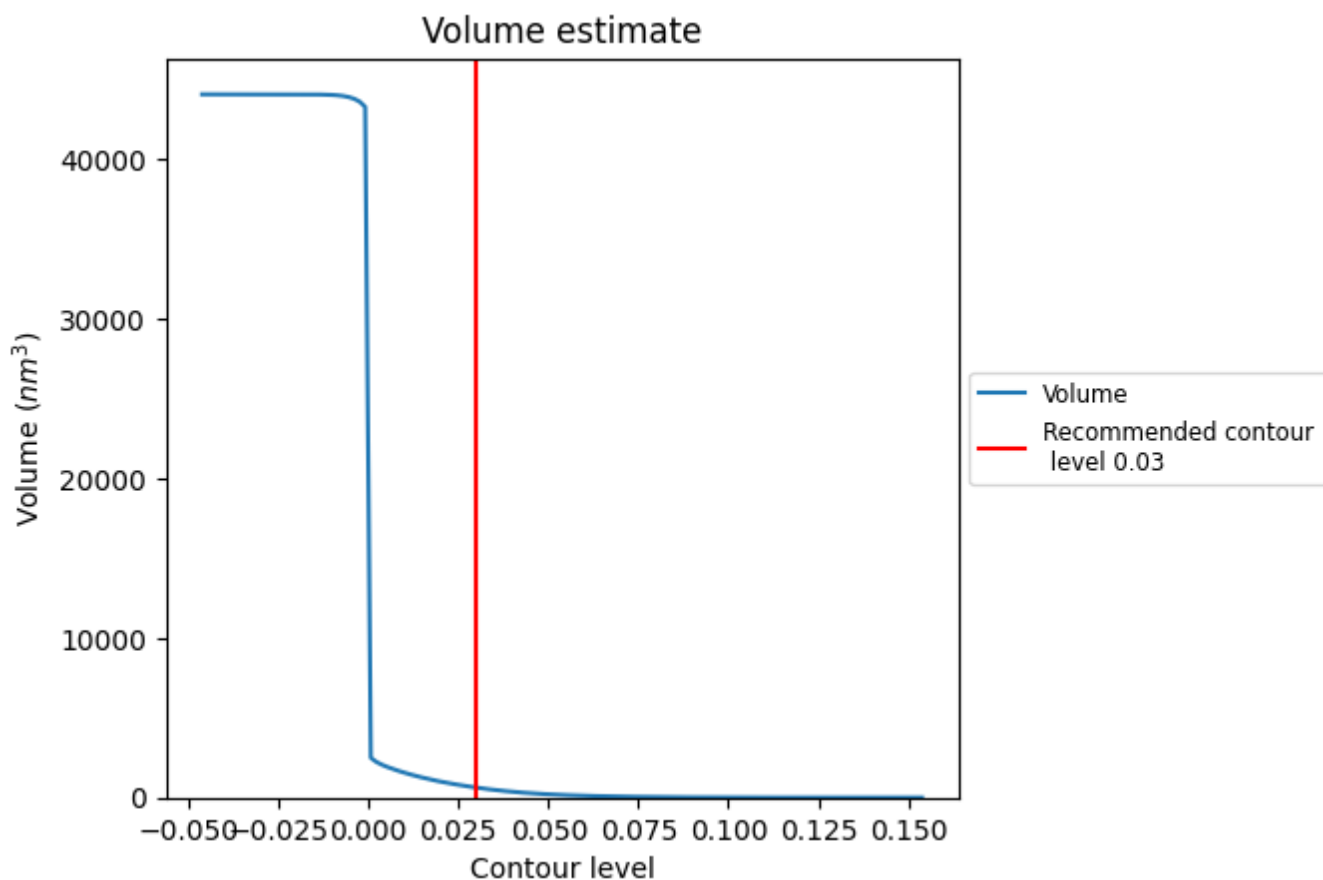
This section contains the results of statistical analysis of the map.

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.

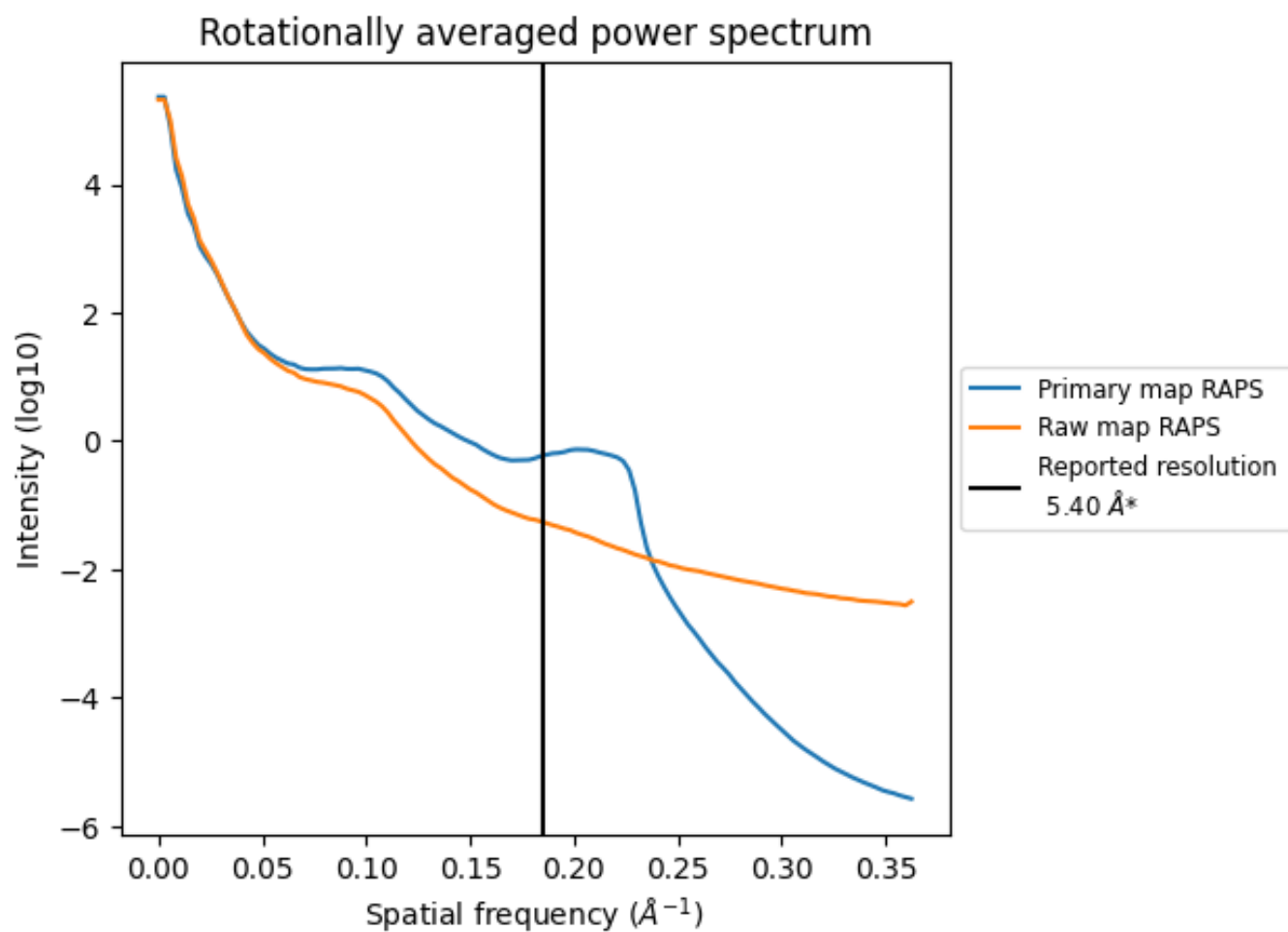
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 624 nm³; this corresponds to an approximate mass of 564 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 [\(i\)](#)

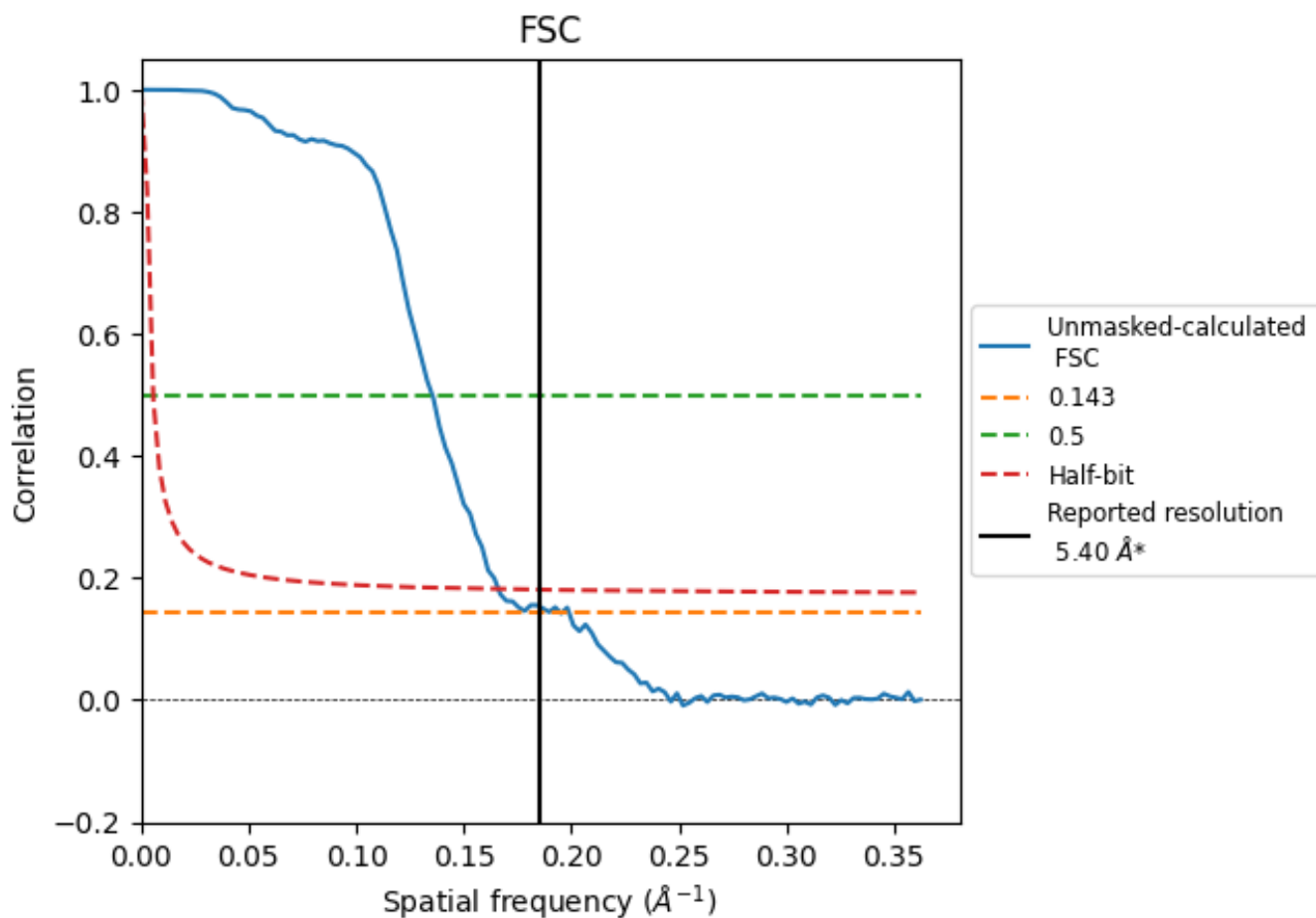


*Reported resolution corresponds to spatial frequency of 0.185 Å⁻¹

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 0.185 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.13	7.39	6.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

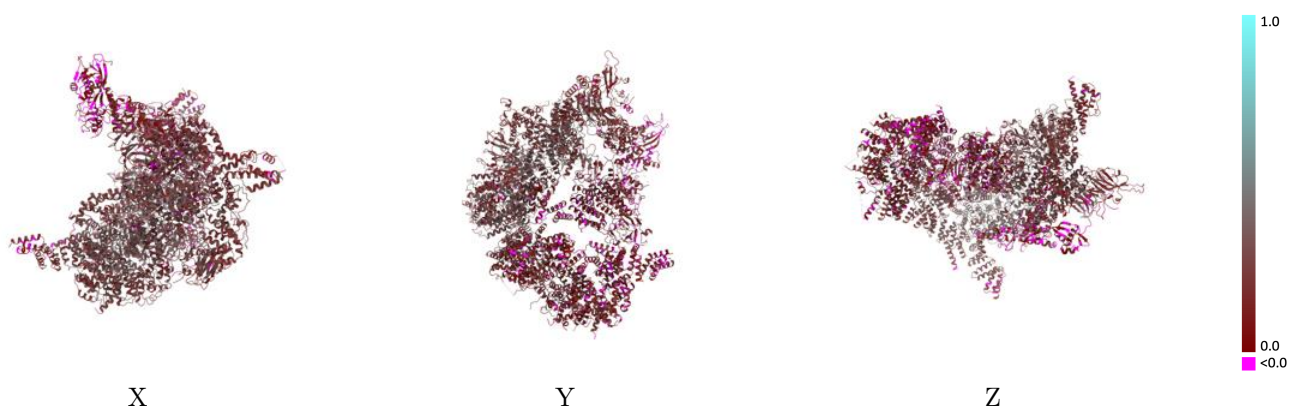
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15201 and PDB model 8A61. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

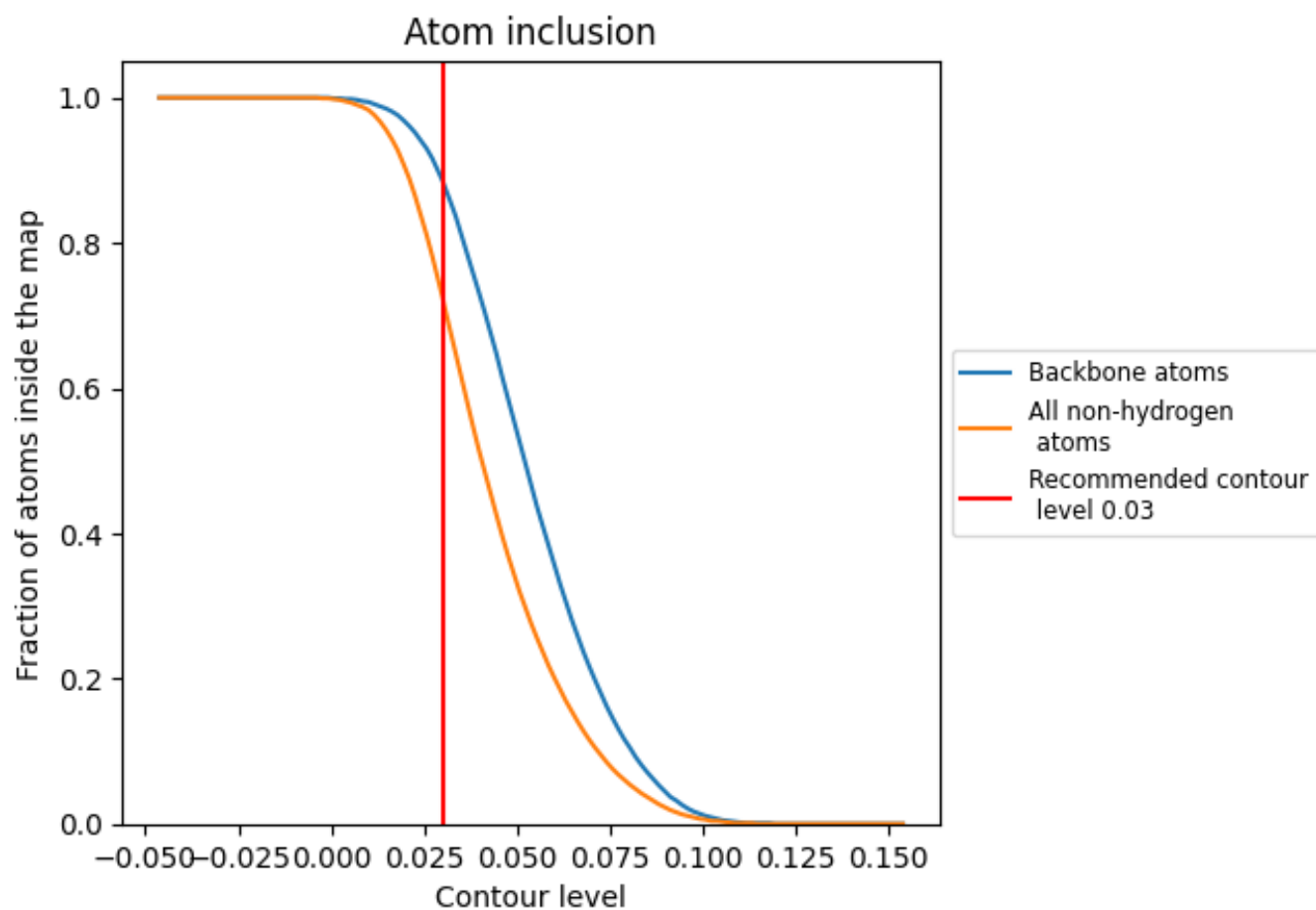


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.





































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 72% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7240	 0.2230
A	 0.6610	 0.1400
C	 0.7560	 0.2260
D	 0.7780	 0.2620
E	 0.4800	 0.1730
F	 0.7260	 0.2040
G	 0.6970	 0.2430
H	 0.6080	 0.1490
I	 0.7030	 0.2690
J	 0.7640	 0.2280
K	 0.6510	 0.1730
N	 0.7150	 0.3220
O	 0.8120	 0.3160
P	 0.8120	 0.2600
Q	 0.7870	 0.2650
T	 0.6550	 0.1730
U	 0.3870	 0.0540
W	 0.1930	 0.1230

