



wwPDB EM Validation Summary Report ⓘ

Jul 20, 2023 – 01:45 am BST

PDB ID : 8A5Y
EMDB ID : EMD-15199
Title : *S. cerevisiae* apo unphosphorylated APC/C.
Authors : Barford, D.; Fernandez-Vazquez, E.; Zhang, Z.; Yang, J.
Deposited on : 2022-06-16
Resolution : 4.90 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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

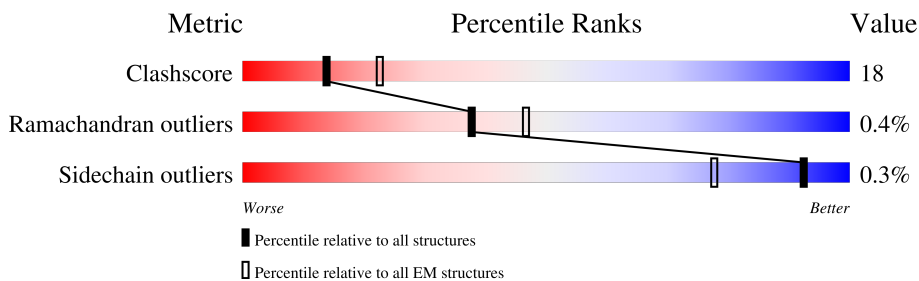
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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	F	758	
1	H	758	
2	J	850	
2	K	850	
3	G	124	
3	W	124	
4	E	265	
5	T	853	

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Mol	Chain	Length	Quality of chain
6	U	165	
7	C	1748	
8	O	685	
9	D	626	
9	P	626	
10	I	170	
11	N	368	
12	Q	652	
13	A	250	

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 57866 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	Total	C	N	O	S	0	0
			3991	2569	656	739	27		
1	H	505	Total	C	N	O	S	0	0
			4038	2599	664	748	27		

- 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	Total	C	N	O	S	0	0
			4124	2658	674	769	23		
2	K	505	Total	C	N	O	S	0	0
			4102	2642	673	764	23		

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
3	G	35	Total	C	N	O	S	0	0
			284	174	51	58	1		
3	W	35	Total	C	N	O	S	0	0
			284	174	51	58	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
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
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
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
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
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
10	I	111	Total	C	N	O	S	0	0
			906	568	158	176	4		

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

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

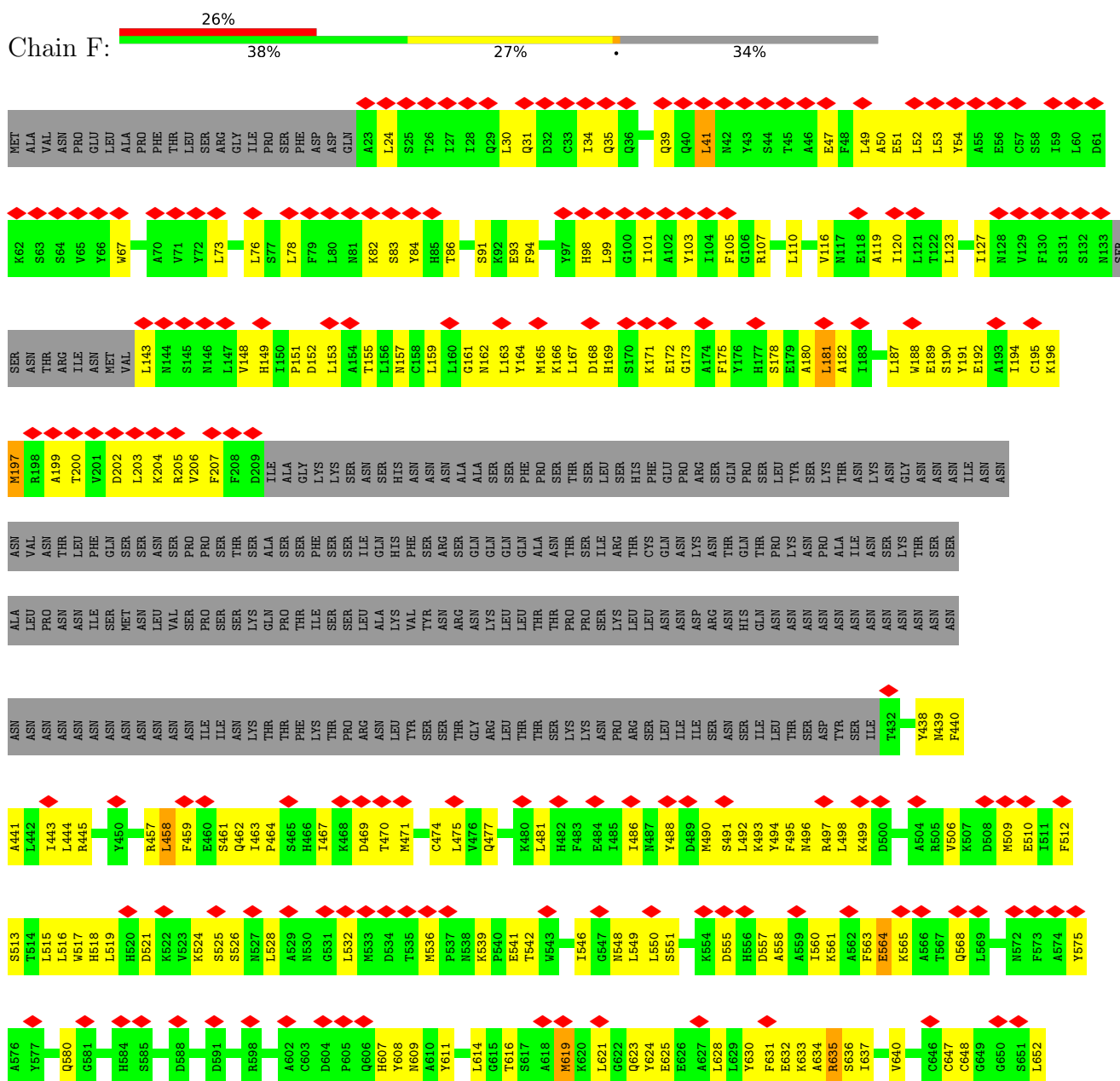
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

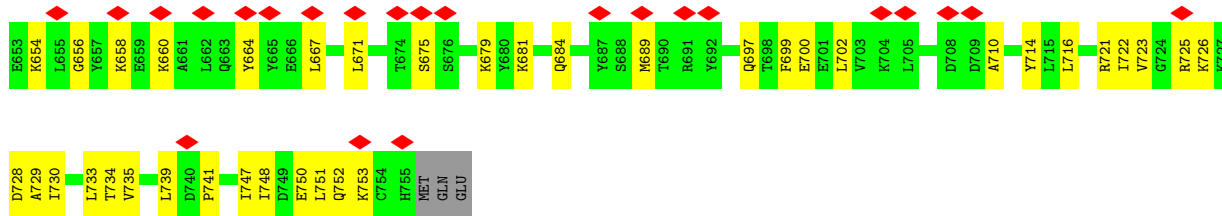
Mol	Chain	Residues	Atoms		AltConf
14	U	3	Total	Zn	0
			3	3	

3 Residue-property plots

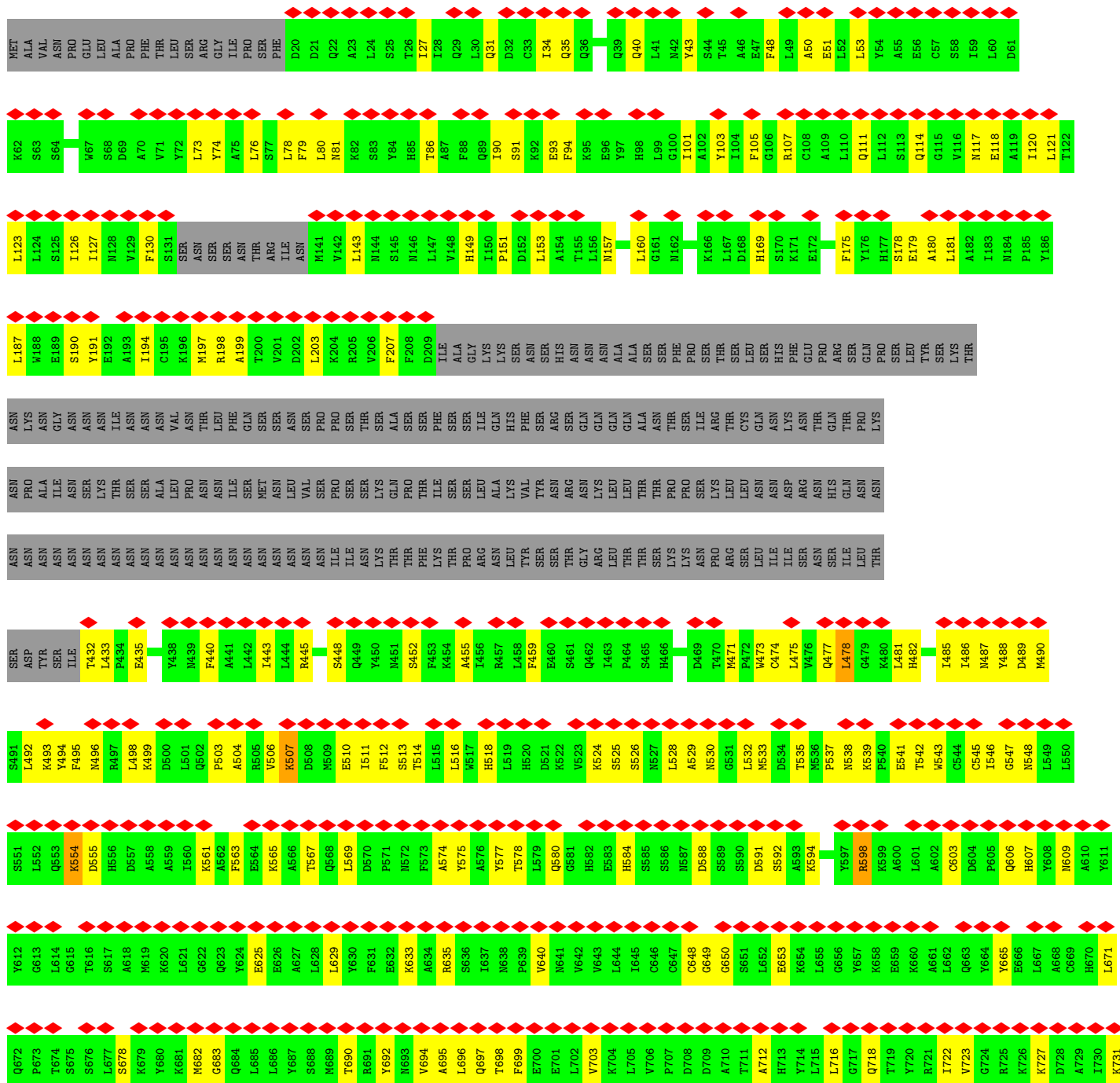
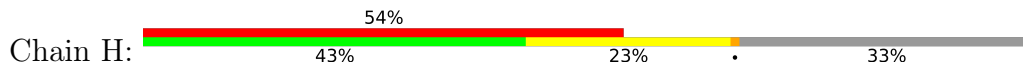
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

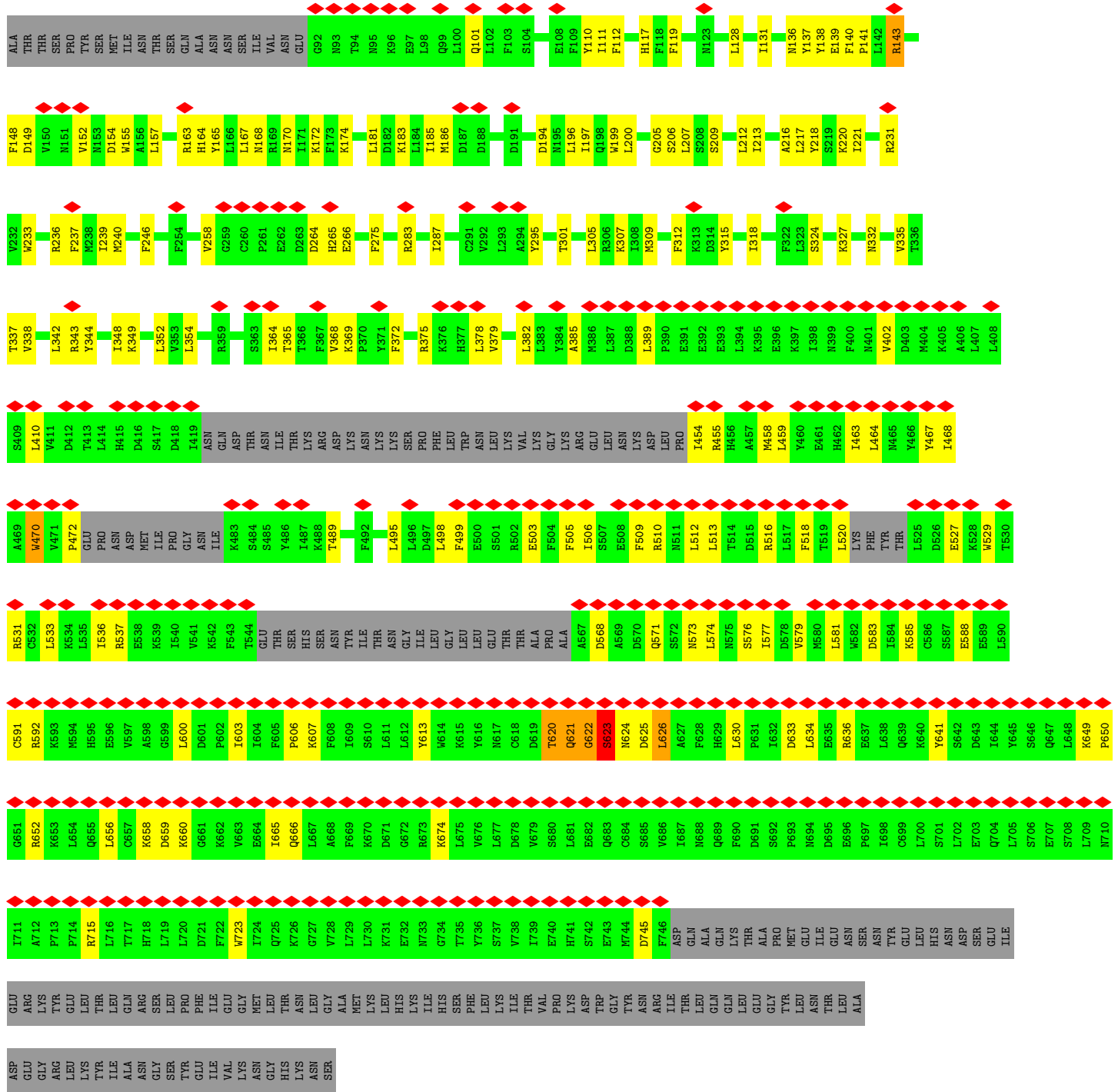
- Molecule 1: Anaphase-promoting complex subunit CDC27



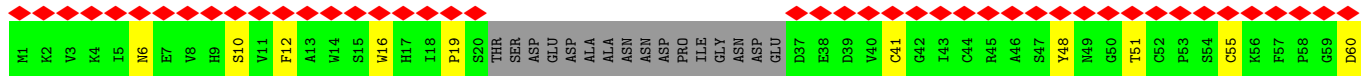


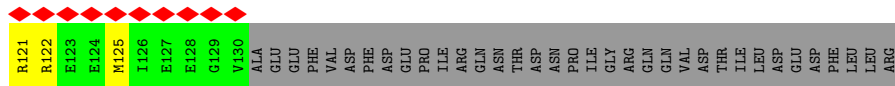
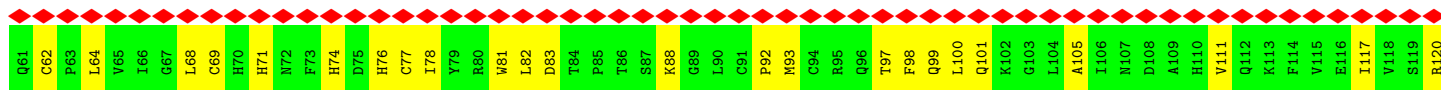
• Molecule 1: Anaphase-promoting complex subunit CDC27



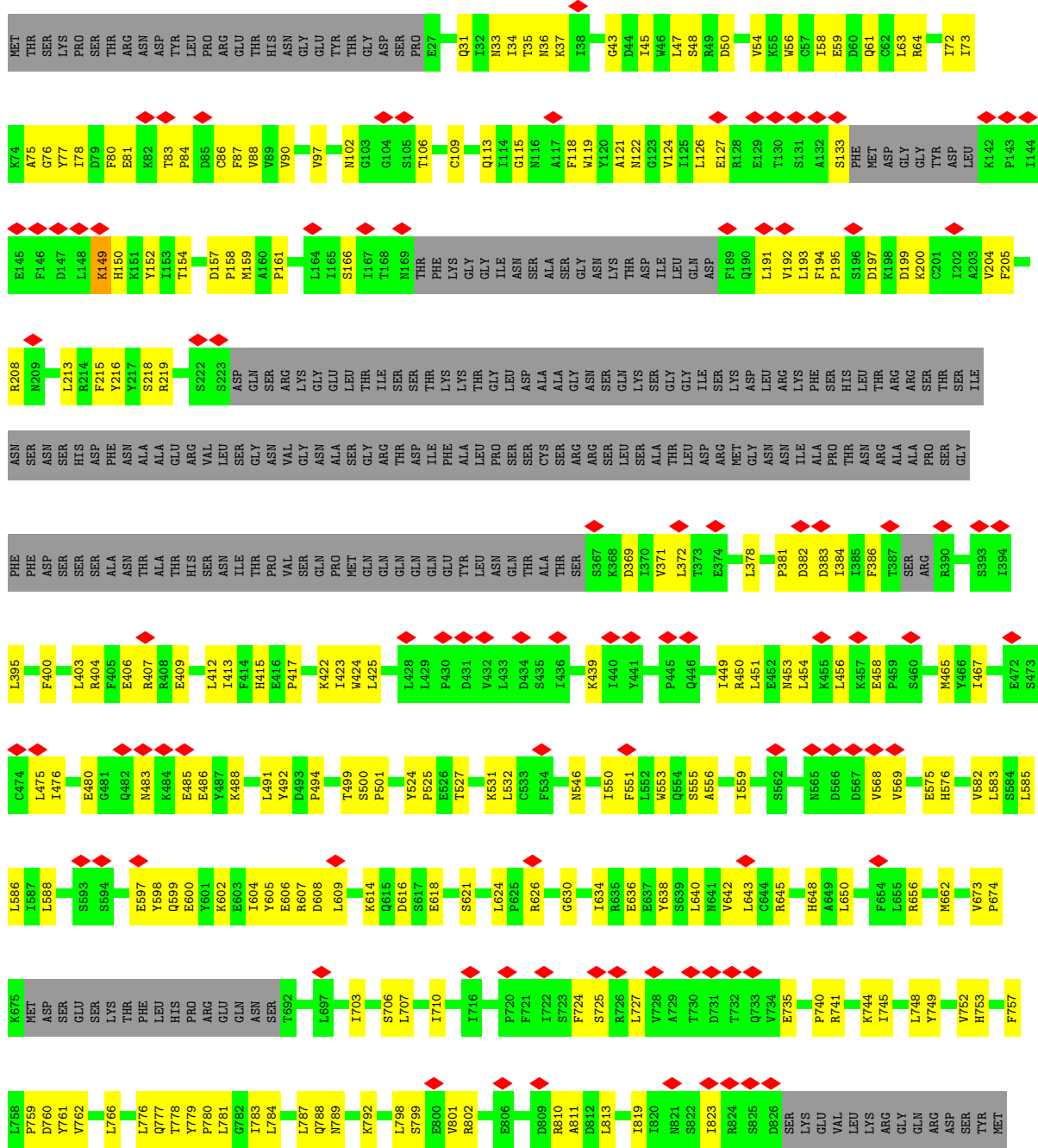


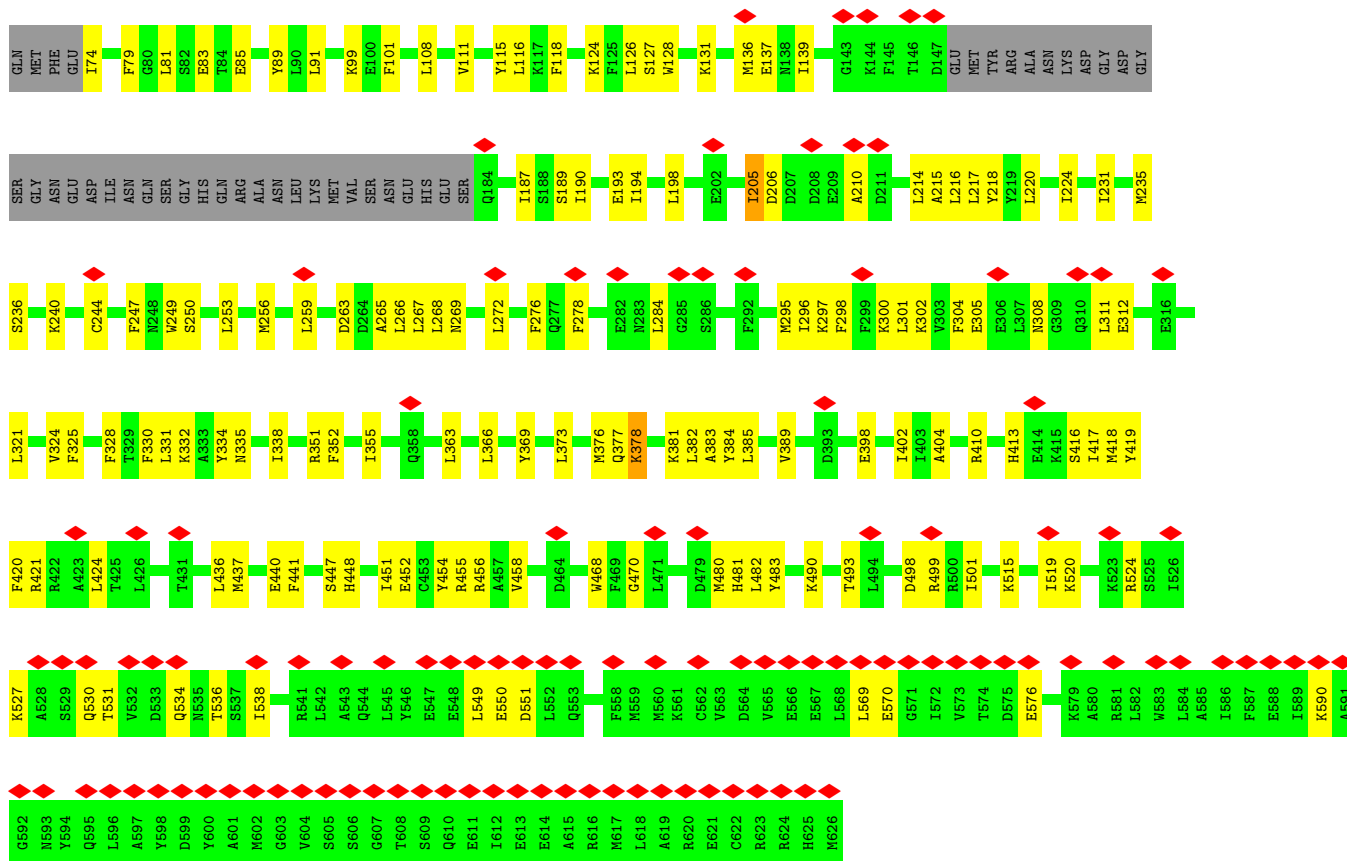
• Molecule 6: Anaphase-promoting complex subunit 11



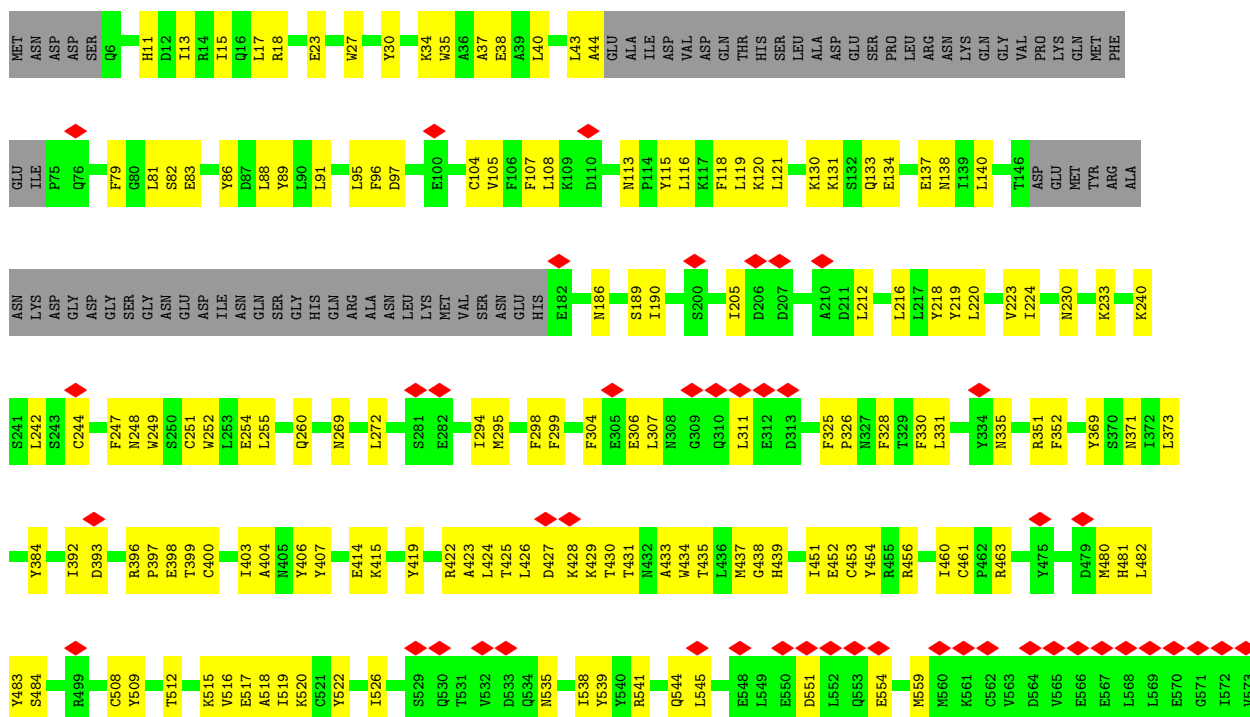


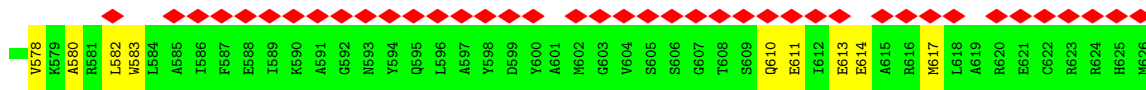
• Molecule 7: Anaphase-promoting complex subunit 1



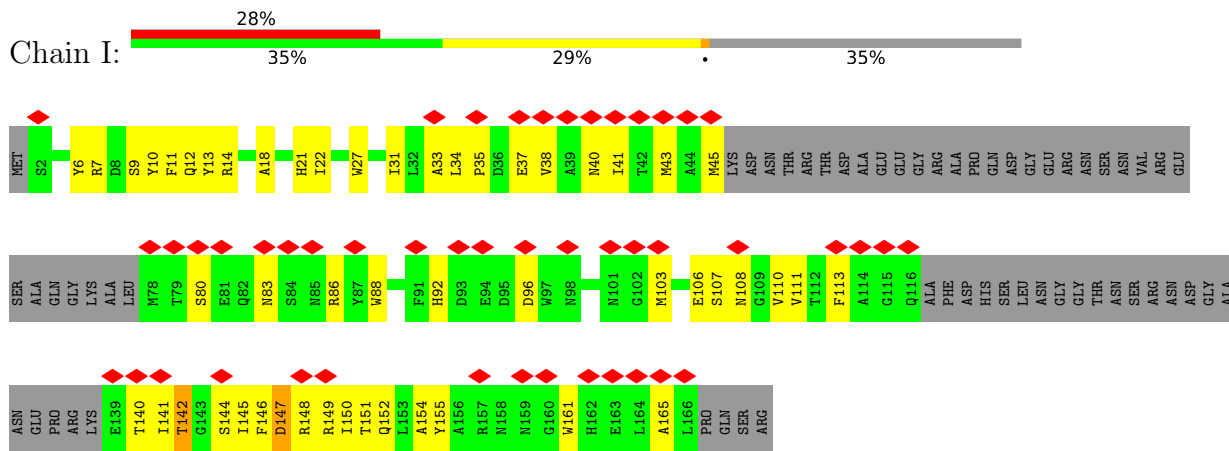


● Molecule 9: Anaphase-promoting complex subunit CDC23

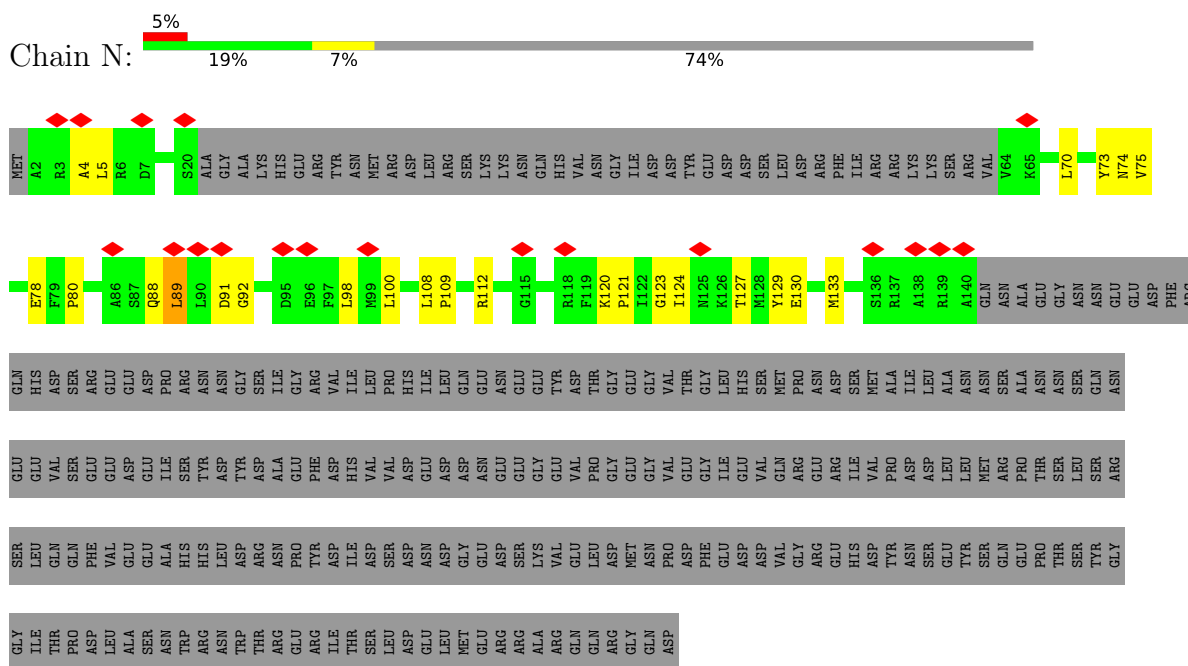




• Molecule 10: Anaphase-promoting complex subunit SWM1

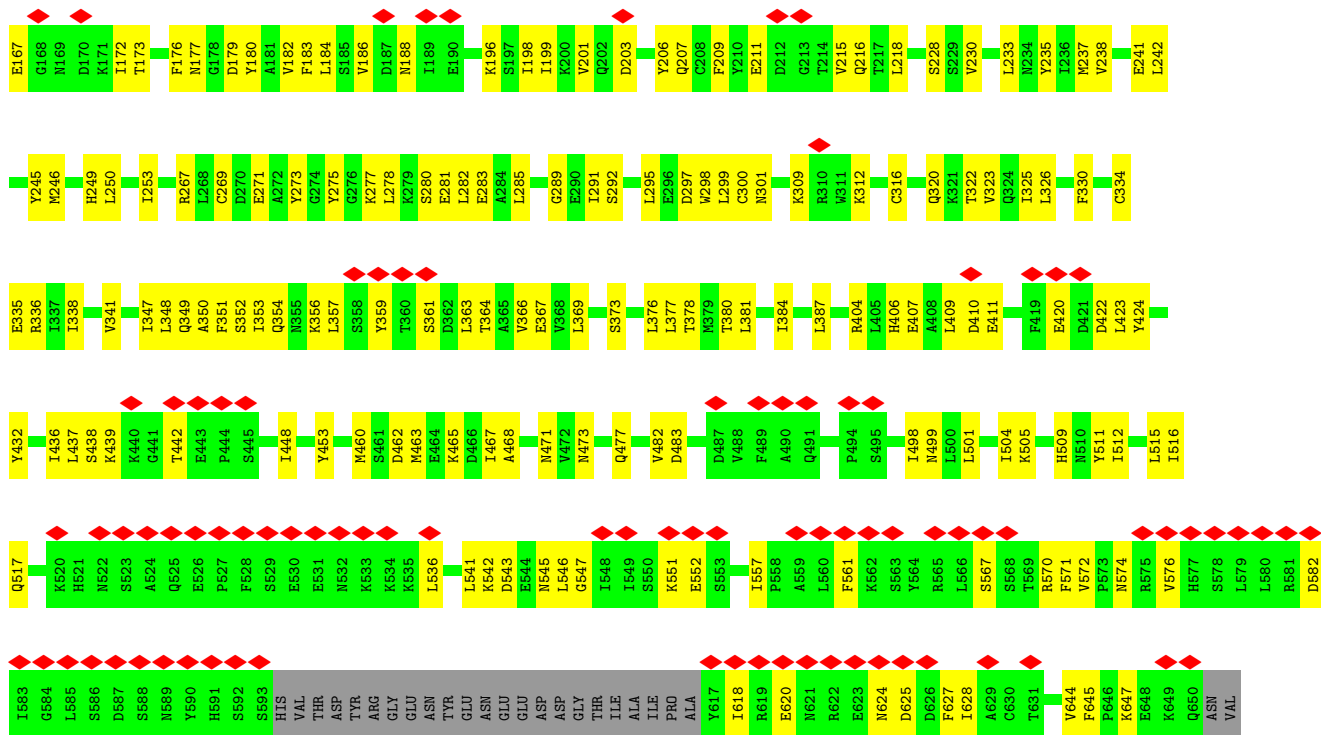


• Molecule 11: Anaphase-promoting complex subunit MND2

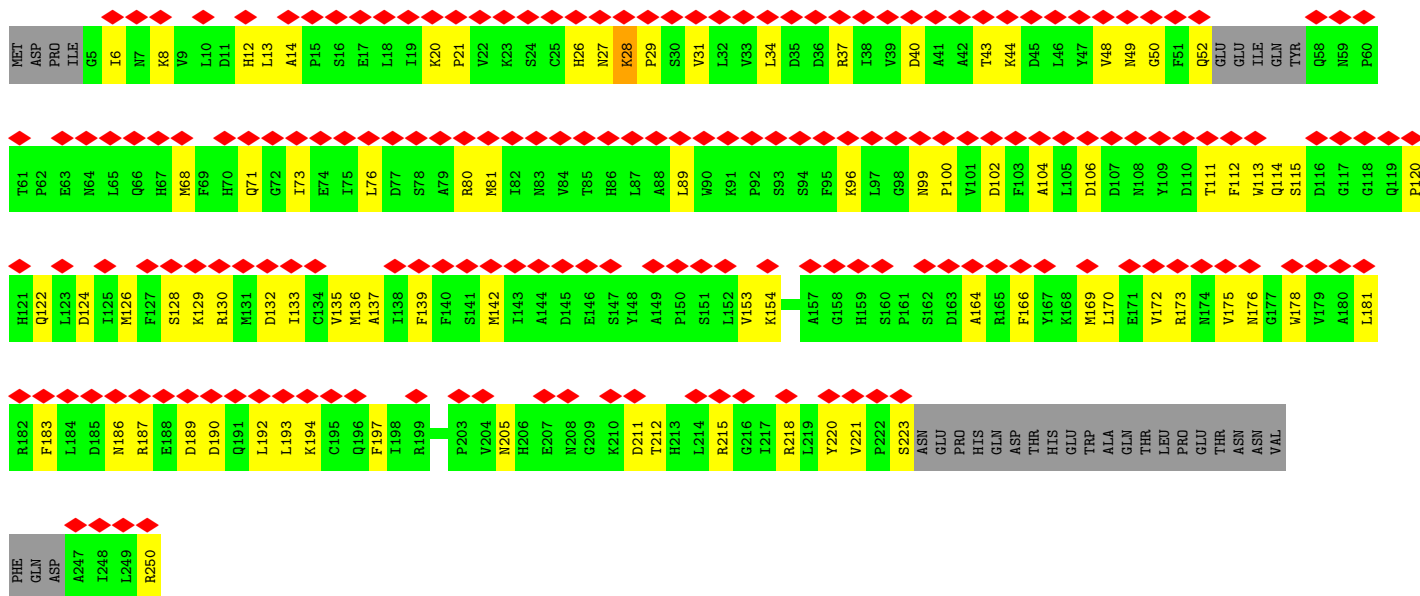
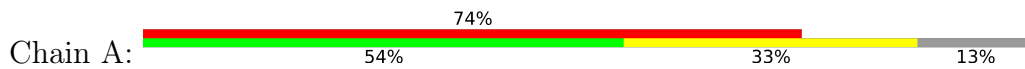


• Molecule 12: Anaphase-promoting complex subunit 4





● 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	372535	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)	9000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.38, 1.38, 1.38	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

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	0.31	0/4079	0.60	7/5525 (0.1%)
1	H	0.28	0/4126	0.53	1/5585 (0.0%)
2	J	0.30	0/4210	0.61	5/5688 (0.1%)
2	K	0.30	0/4188	0.57	0/5657
3	G	0.28	0/285	0.76	0/384
3	W	0.27	0/285	0.58	0/384
4	E	0.29	0/1108	0.60	1/1481 (0.1%)
5	T	0.26	0/5479	0.53	1/7420 (0.0%)
6	U	0.26	0/936	0.57	0/1265
7	C	0.28	0/11057	0.58	4/15038 (0.0%)
8	O	0.29	0/5384	0.58	0/7287
9	D	0.28	0/4621	0.56	2/6243 (0.0%)
9	P	0.27	0/4618	0.55	0/6231
10	I	0.32	0/930	0.66	0/1263
11	N	0.27	0/800	0.64	1/1076 (0.1%)
12	Q	0.27	0/5193	0.53	0/7024
13	A	0.25	0/1780	0.56	0/2411
All	All	0.28	0/59079	0.57	22/79962 (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	4
7	C	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	752	LEU	CB-CG-CD2	-7.79	97.76	111.00
7	C	1363	LEU	CA-CB-CG	6.89	131.16	115.30
2	J	482	CYS	CA-CB-SG	6.65	125.98	114.00
1	F	458	LEU	CA-CB-CG	6.61	130.51	115.30
1	F	181	LEU	CA-CB-CG	-6.18	101.08	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	1551	PRO	Peptide
5	T	620	THR	Peptide
5	T	621	GLN	Peptide
5	T	622	GLY	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	183	0
1	H	4038	0	4010	141	0
2	J	4124	0	4085	186	0
2	K	4102	0	4065	184	0
3	G	284	0	293	19	0
3	W	284	0	293	21	0
4	E	1091	0	1058	38	0
5	T	5362	0	5336	157	0
6	U	912	0	873	31	0
7	C	10832	0	10637	435	0
8	O	5285	0	5290	235	0
9	D	4524	0	4391	139	0
9	P	4520	0	4415	143	0
10	I	906	0	813	60	0
11	N	784	0	784	24	0
12	Q	5086	0	5095	180	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	1738	0	1705	59	0
14	U	3	0	0	0	0
All	All	57866	0	57090	2031	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 18.

The worst 5 of 2031 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)
5:T:463:ILE:HG12	7:C:1412:TYR:HE1	1.24	1.02
7:C:78:ILE:HD13	7:C:119:TRP:HD1	1.30	0.95
7:C:902:ALA:HA	7:C:905:ILE:HG12	1.49	0.92
9:P:95:LEU:HD11	9:P:104:CYS:HB2	1.53	0.91
2:K:453:LEU:HD12	2:K:459:LEU:HD23	1.52	0.90

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%)	479 (97%)	17 (3%)	0	100	100
1	H	499/758 (66%)	483 (97%)	13 (3%)	3 (1%)	25	65
2	J	505/850 (59%)	488 (97%)	17 (3%)	0	100	100
2	K	501/850 (59%)	487 (97%)	14 (3%)	0	100	100
3	G	33/124 (27%)	33 (100%)	0	0	100	100
3	W	33/124 (27%)	33 (100%)	0	0	100	100
4	E	120/265 (45%)	118 (98%)	2 (2%)	0	100	100
5	T	638/853 (75%)	613 (96%)	19 (3%)	6 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	U	110/165 (67%)	108 (98%)	1 (1%)	1 (1%)	17	56
7	C	1380/1748 (79%)	1287 (93%)	87 (6%)	6 (0%)	34	72
8	O	654/685 (96%)	625 (96%)	26 (4%)	3 (0%)	29	68
9	D	554/626 (88%)	536 (97%)	15 (3%)	3 (0%)	29	68
9	P	550/626 (88%)	527 (96%)	23 (4%)	0	100	100
10	I	105/170 (62%)	94 (90%)	10 (10%)	1 (1%)	15	54
11	N	92/368 (25%)	89 (97%)	3 (3%)	0	100	100
12	Q	619/652 (95%)	597 (96%)	21 (3%)	1 (0%)	47	81
13	A	212/250 (85%)	203 (96%)	8 (4%)	1 (0%)	29	68
All	All	7101/9872 (72%)	6800 (96%)	276 (4%)	25 (0%)	38	72

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	588	ASP
5	T	621	GLN
5	T	624	ASN
5	T	745	ASP
7	C	844	VAL

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%)	432 (100%)	1 (0%)	93	96
1	H	440/684 (64%)	439 (100%)	1 (0%)	93	96
2	J	450/760 (59%)	449 (100%)	1 (0%)	93	96
2	K	448/760 (59%)	445 (99%)	3 (1%)	84	90
3	G	34/115 (30%)	34 (100%)	0	100	100
3	W	34/115 (30%)	34 (100%)	0	100	100
4	E	123/246 (50%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	T	608/804 (76%)	606 (100%)	2 (0%)	92	95
6	U	103/149 (69%)	103 (100%)	0	100	100
7	C	1177/1568 (75%)	1174 (100%)	3 (0%)	92	95
8	O	597/643 (93%)	594 (100%)	3 (0%)	88	93
9	D	477/560 (85%)	475 (100%)	2 (0%)	91	94
9	P	477/560 (85%)	475 (100%)	2 (0%)	91	94
10	I	95/144 (66%)	93 (98%)	2 (2%)	53	72
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%)	188 (99%)	2 (1%)	73	85
All	All	6341/8948 (71%)	6319 (100%)	22 (0%)	92	95

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	D	14	ARG
9	P	371	ASN
9	P	138	ASN
10	I	147	ASP
5	T	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
8	O	61	ASN
12	Q	320	GLN
8	O	333	ASN
9	P	535	ASN
8	O	220	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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](#)

There are no chain breaks in this entry.

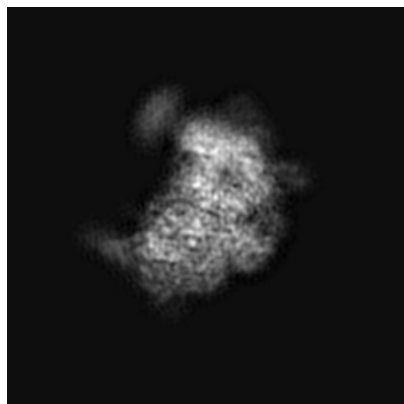
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15199. These allow visual inspection of the internal detail of the map and identification of artifacts.

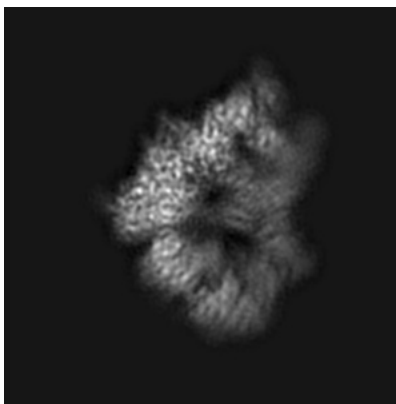
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

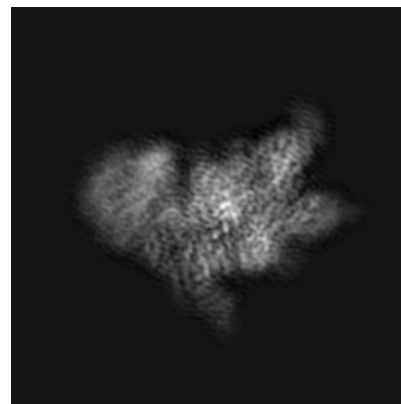
6.1.1 Primary map



X

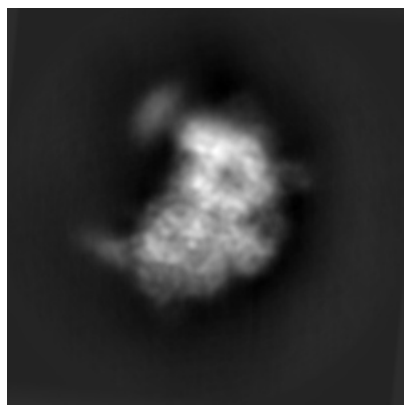


Y

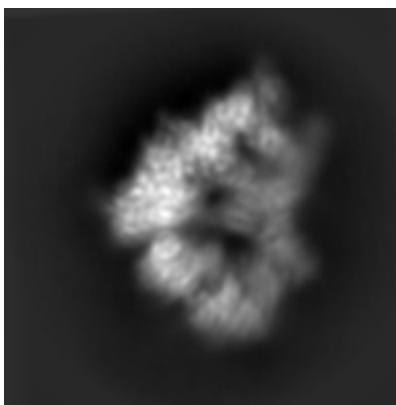


Z

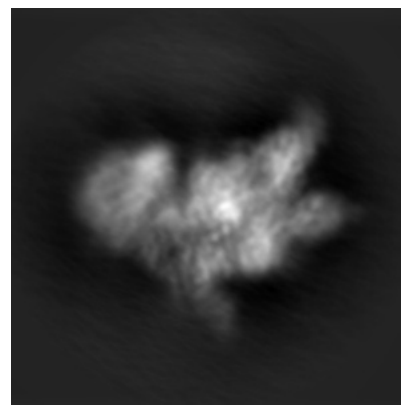
6.1.2 Raw map



X



Y

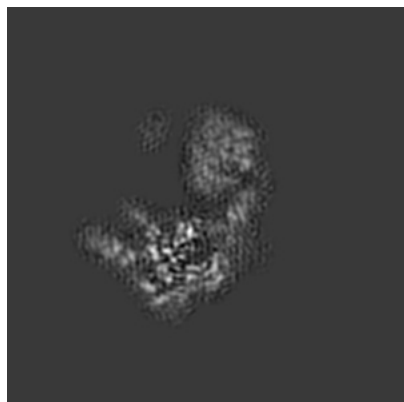


Z

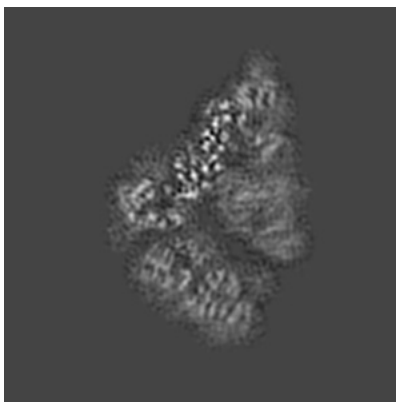
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

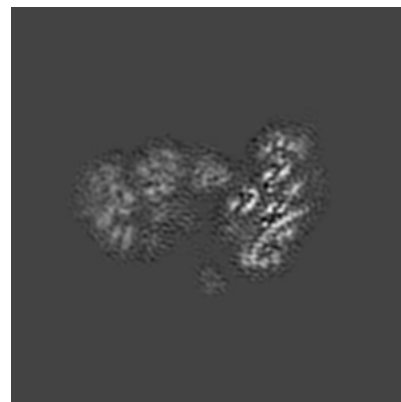
6.2.1 Primary map



X Index: 128

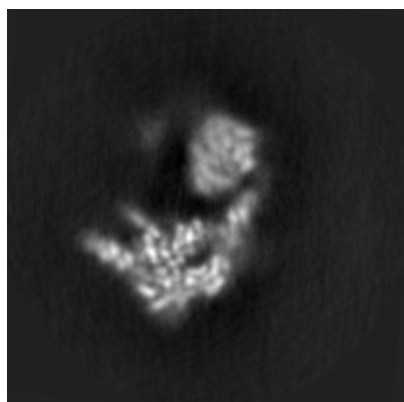


Y Index: 128

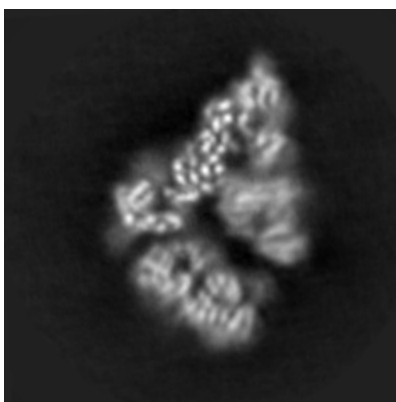


Z Index: 128

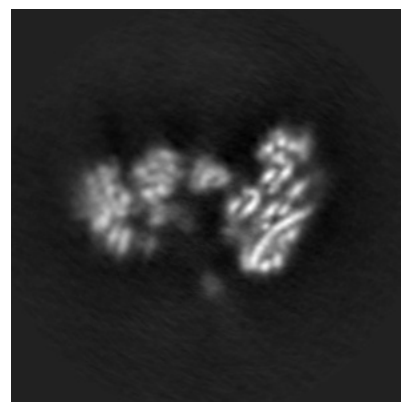
6.2.2 Raw map



X Index: 128



Y Index: 128

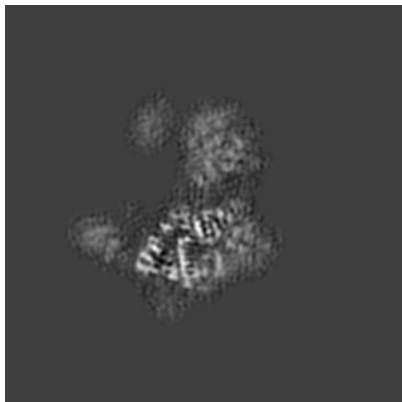


Z Index: 128

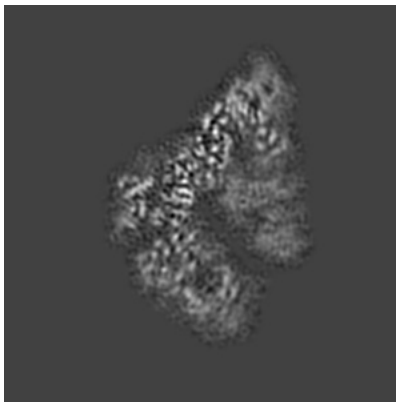
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

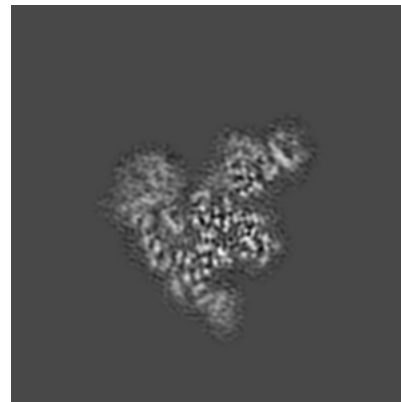
6.3.1 Primary map



X Index: 137

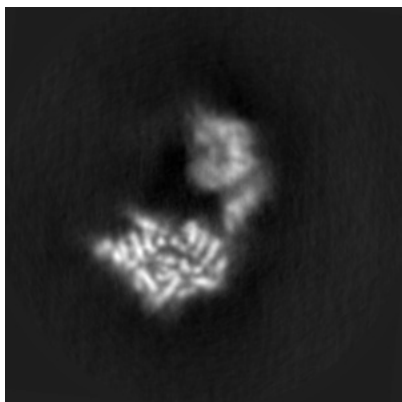


Y Index: 122

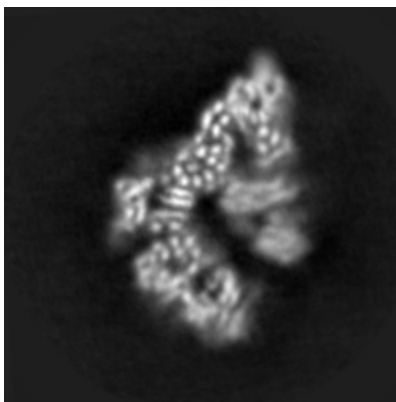


Z Index: 105

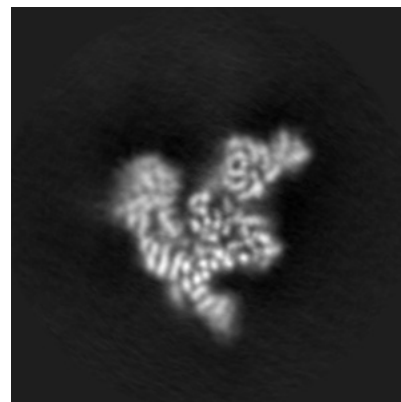
6.3.2 Raw map



X Index: 123



Y Index: 123

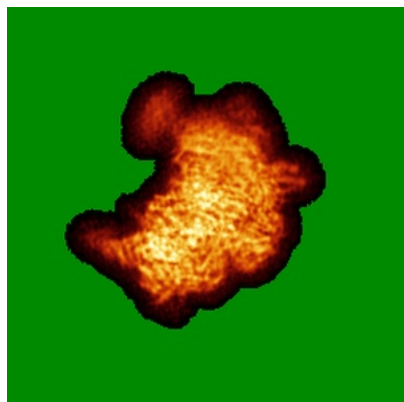


Z Index: 103

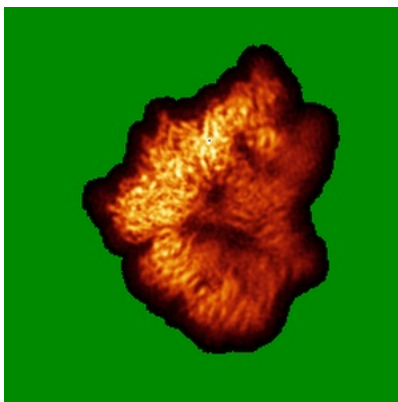
The images above show the largest variance slices of the map in three orthogonal directions.

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

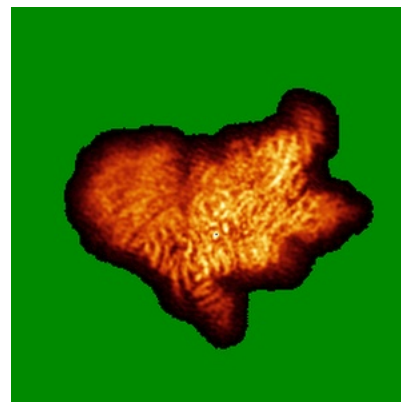
6.4.1 Primary map



X

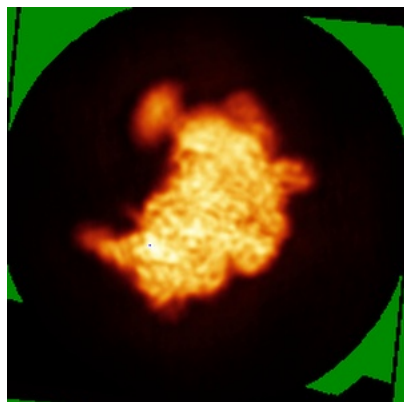


Y

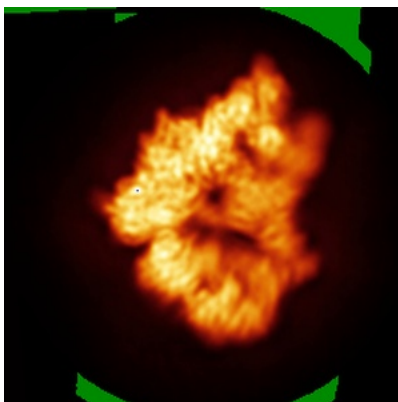


Z

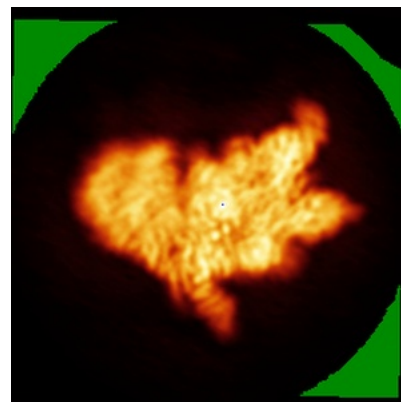
6.4.2 Raw map



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.

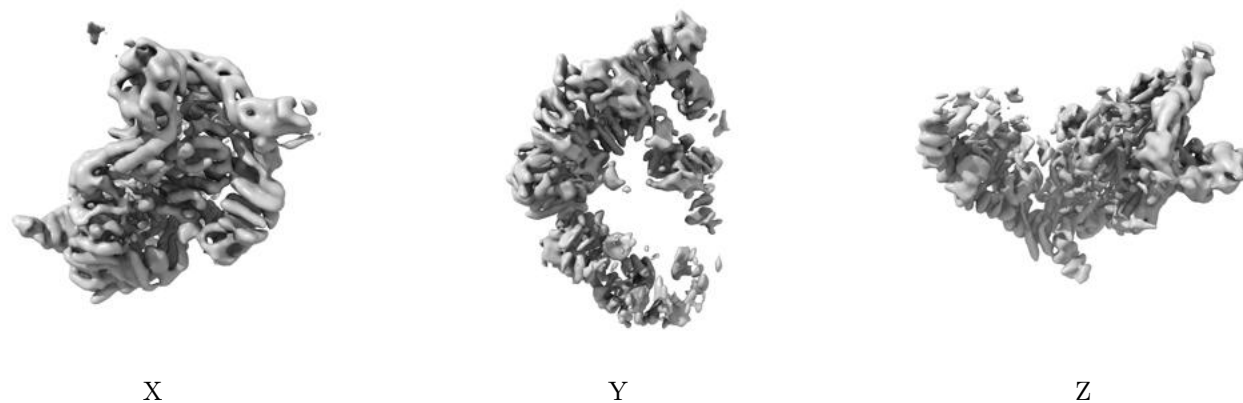
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

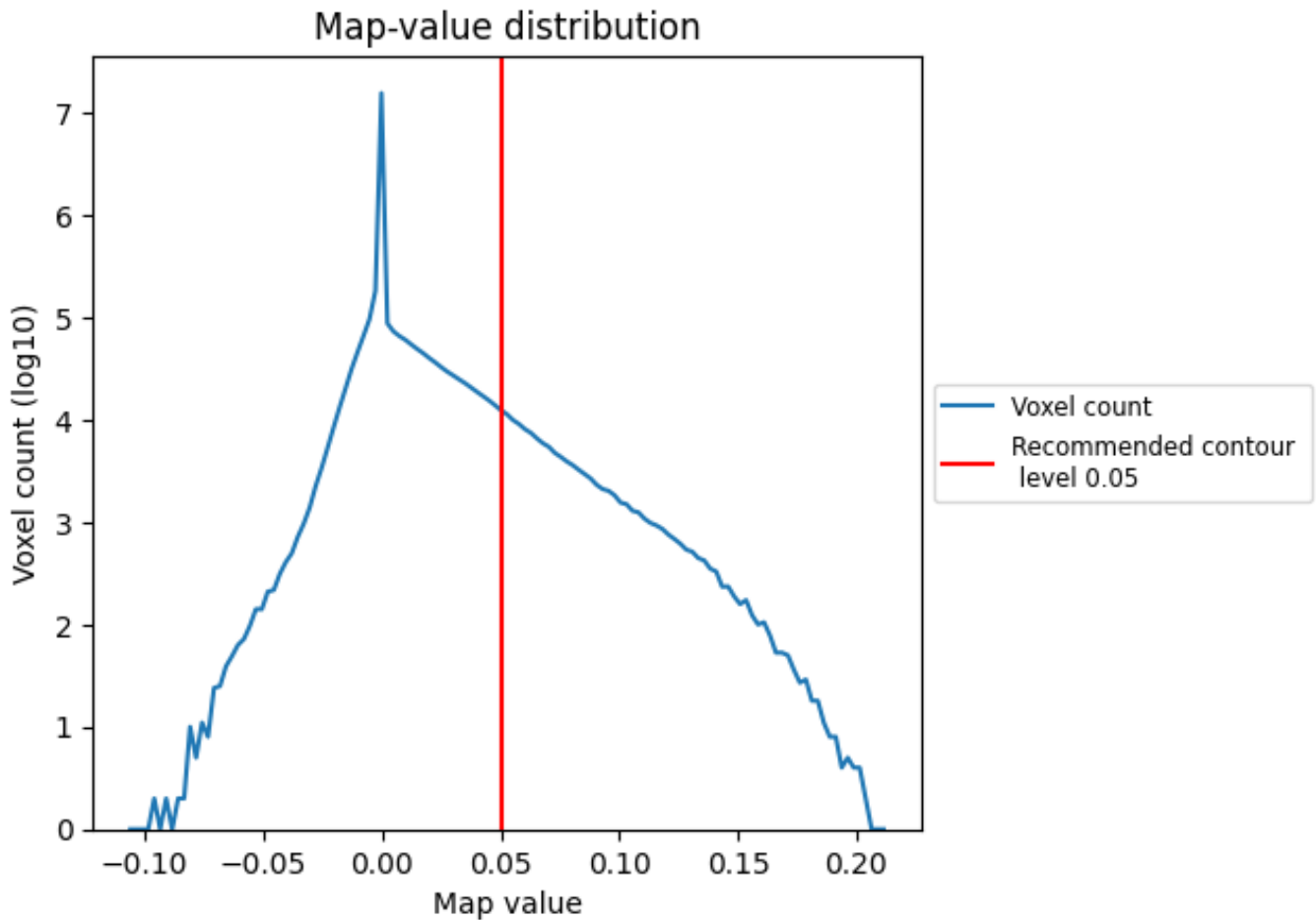
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

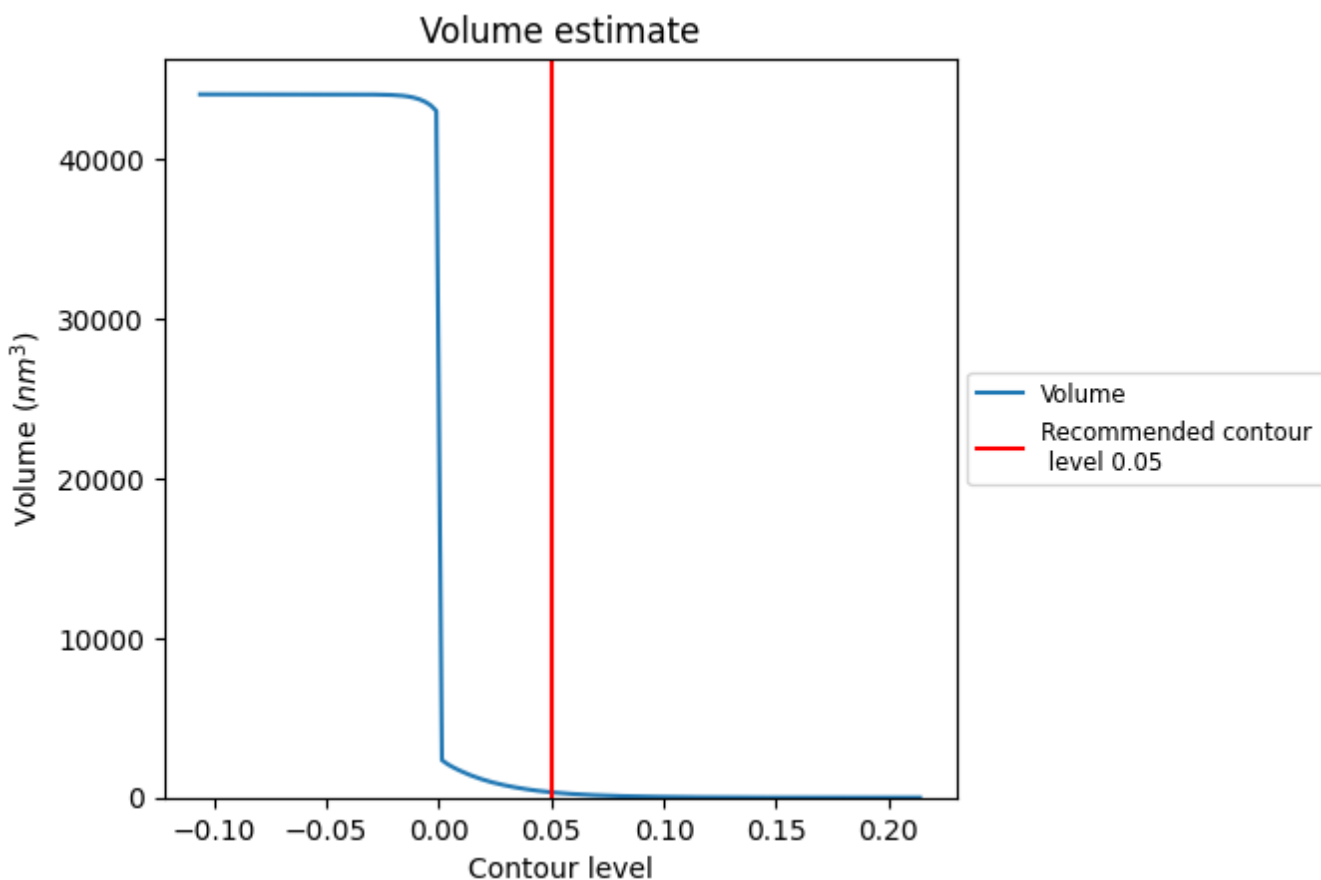
This section contains the results of statistical analysis of the map.

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.

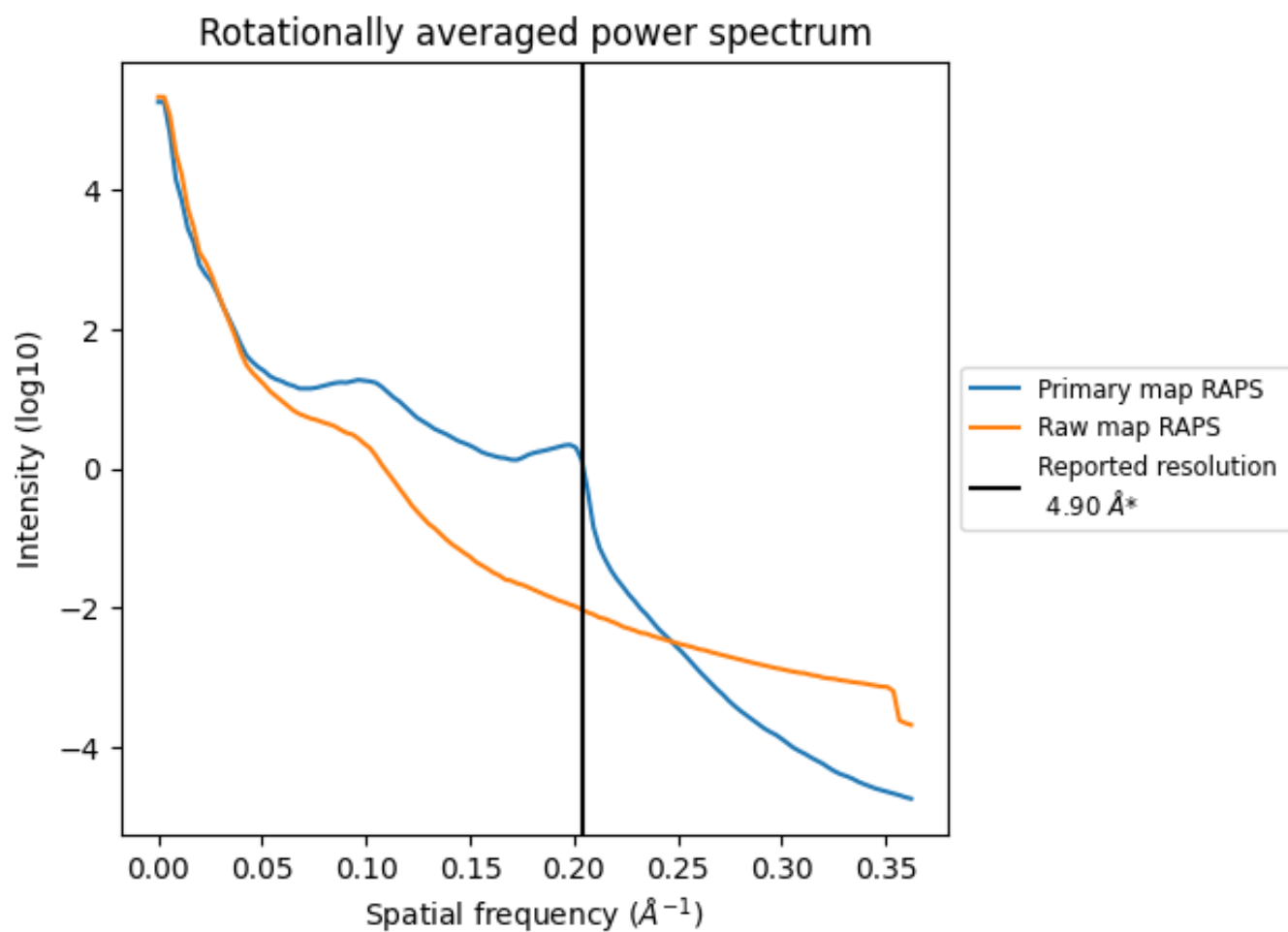
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 332 nm³; this corresponds to an approximate mass of 300 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

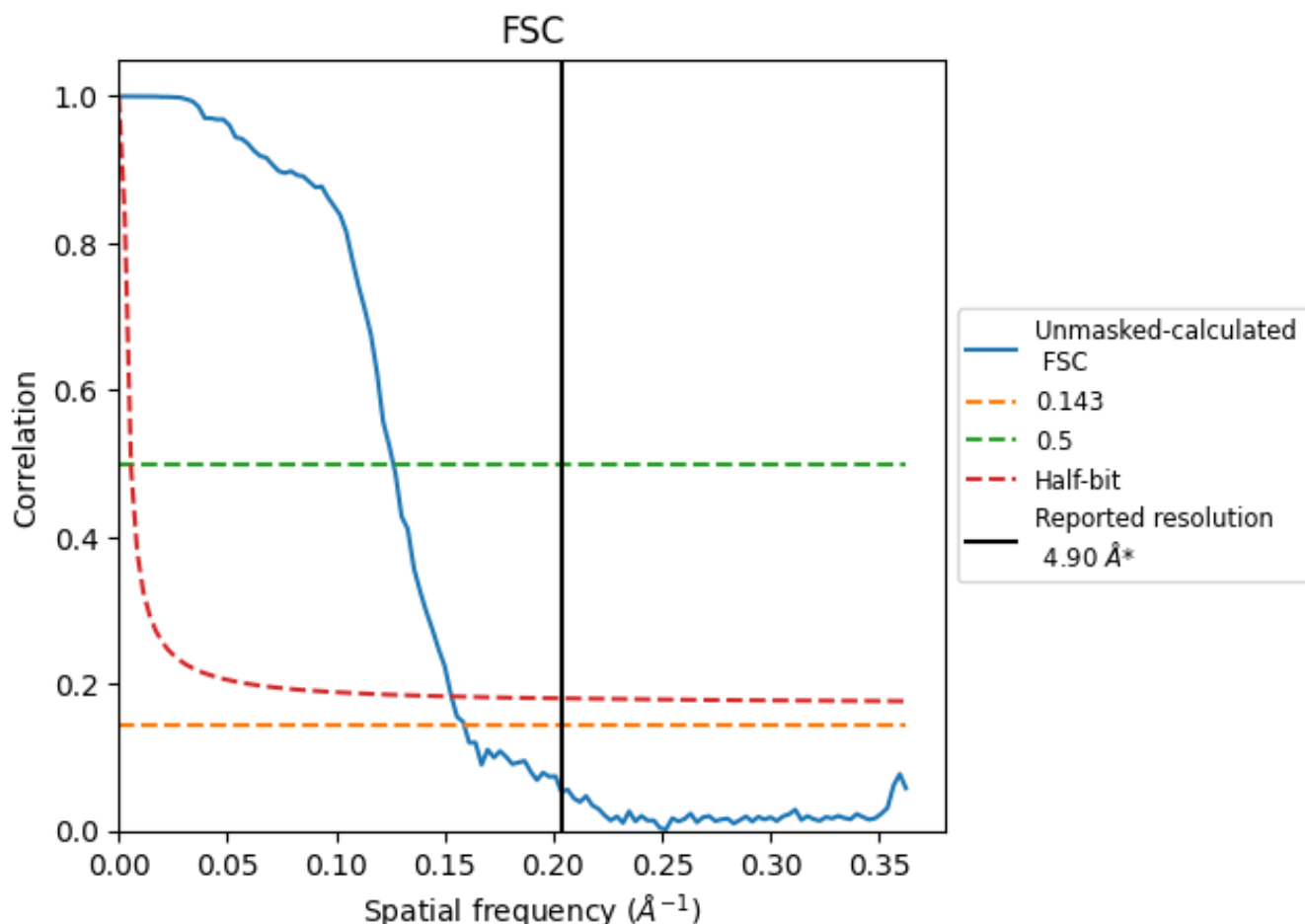


*Reported resolution corresponds to spatial frequency of 0.204 Å⁻¹

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 0.204 Å⁻¹

8.2 Resolution estimates [i](#)

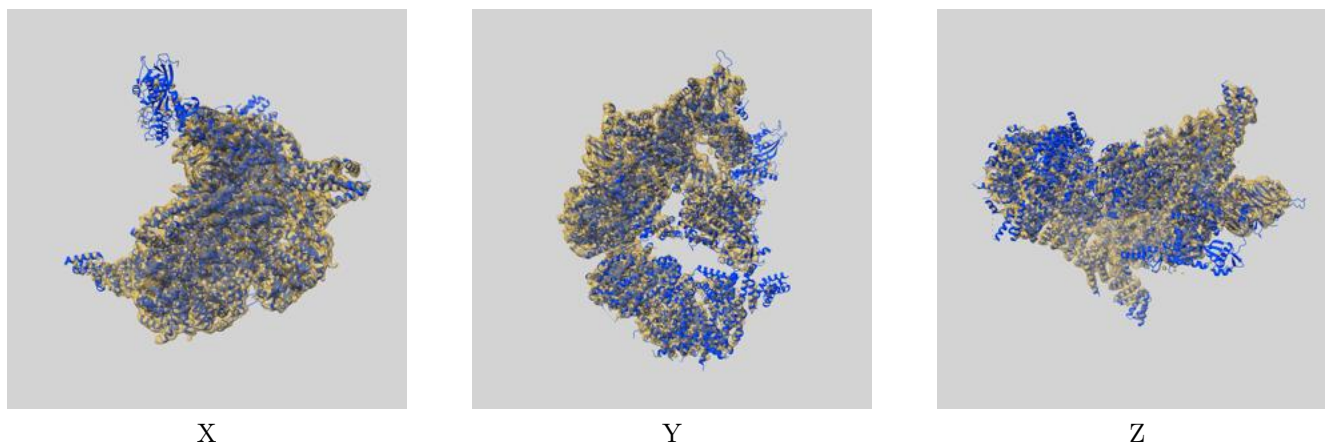
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.29	7.92	6.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.29 differs from the reported value 4.9 by more than 10 %

9 Map-model fit [i](#)

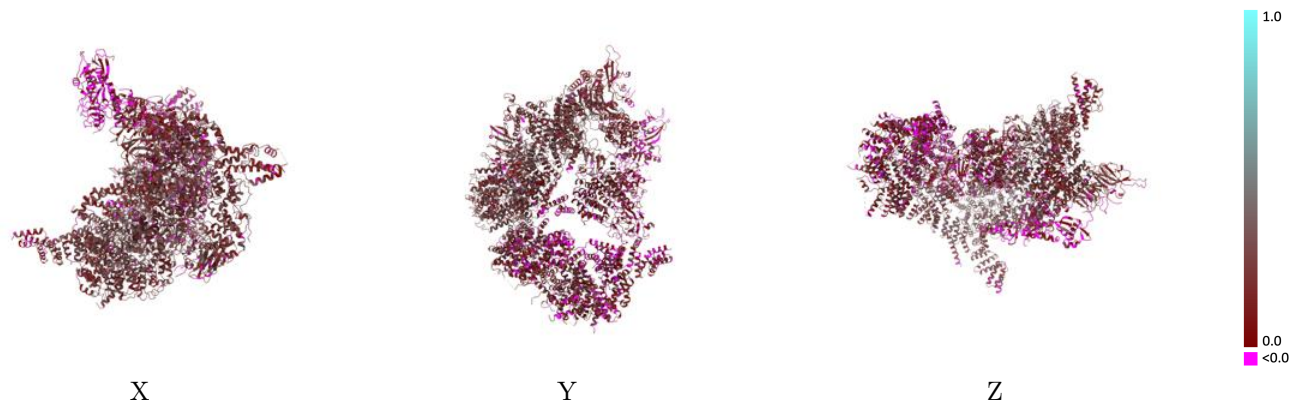
This section contains information regarding the fit between EMDB map EMD-15199 and PDB model 8A5Y. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



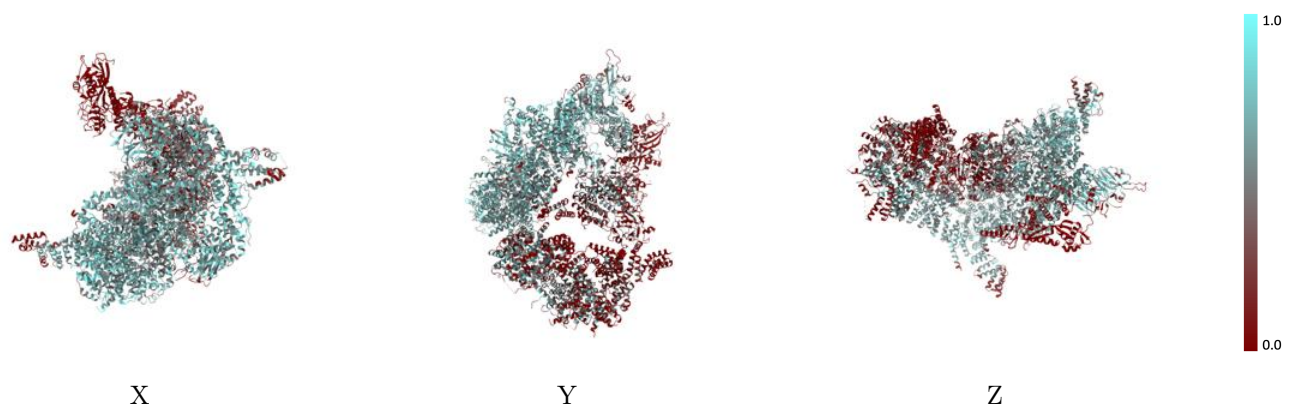
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



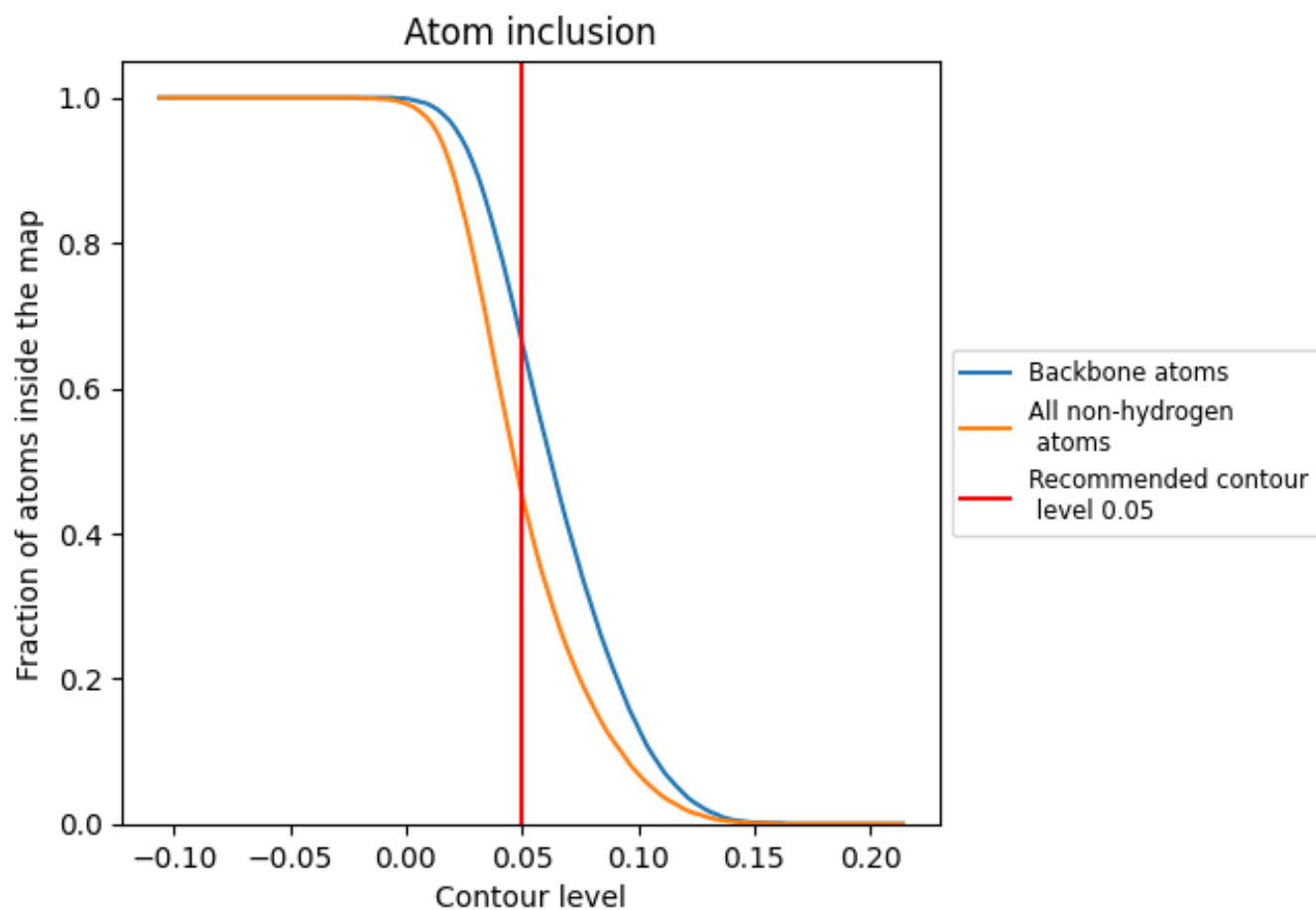
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 45% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4520	 0.1920
A	 0.1560	 0.1200
C	 0.4760	 0.2100
D	 0.5670	 0.2290
E	 0.2190	 0.1580
F	 0.4520	 0.1750
G	 0.5320	 0.2140
H	 0.1840	 0.1270
I	 0.4670	 0.2180
J	 0.5690	 0.2010
K	 0.2380	 0.1160
N	 0.6130	 0.2960
O	 0.6550	 0.2750
P	 0.6030	 0.2300
Q	 0.5890	 0.2310
T	 0.3430	 0.1390
U	 0.0110	 0.0180
W	 0.0070	 0.0220

