wwPDB EM Validation Summary Report

May 4, 2024 – 08:29 am BST

PDB ID	:	8RC4
EMDB ID	:	EMD-19047
Title	:	Structure of Integrator-PP2A complex
Authors	:	Fianu, I.; Ochmann, M.; Walshe, J.L.; Cramer, P.
Deposited on	:	2023-12-06
Resolution	:	3.10 Å(reported)
Based on initial model	:	8RBX

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:

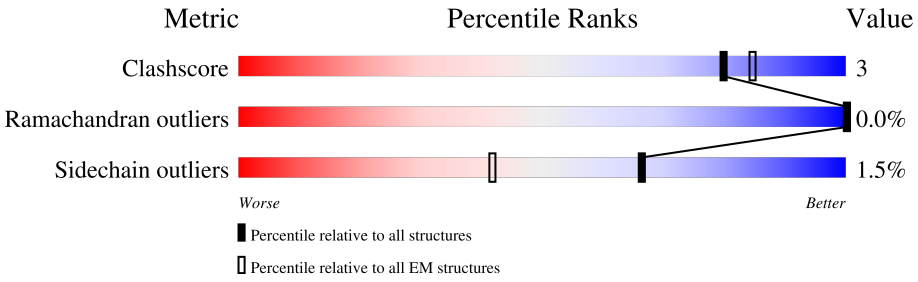
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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 <=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	p	591	96%
2	q	311	92% 7%
3	r	31	97%
4	a	2192	80% 19%
5	b	1204	86% 13%
6	d	963	84% 15%
7	e	1021	84% 14%
8	f	892	62% 37%

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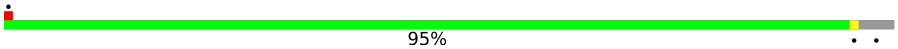
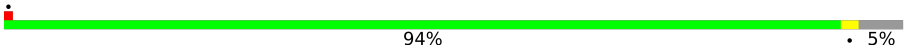
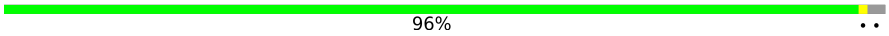
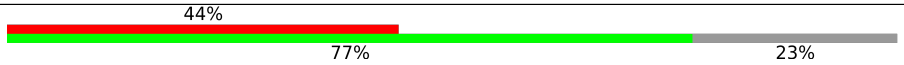
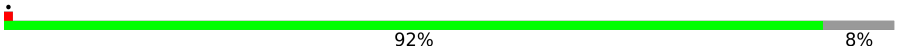
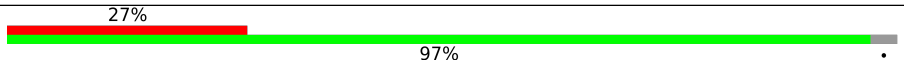
Mol	Chain	Length	Quality of chain
9	g	964	
10	h	995	
11	i	658	
12	k	602	
13	m	706	
14	j	710	
15	n	518	
16	o	451	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 78273 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	p	580	Total	C	N	O	S	0	0
			4437	2828	753	829	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	-1	SER	-	expression tag	UNP P30153
p	0	ASN	-	expression tag	UNP P30153

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	q	290	Total	C	N	O	S	0	0
			2340	1481	405	439	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	-1	SER	-	expression tag	UNP P67775
q	0	ASN	-	expression tag	UNP P67775
q	88	ASN	ASP	engineered mutation	UNP P67775

- Molecule 3 is a protein called DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	r	31	Total	C	N	O	S	0	0
			263	161	44	57	1		

- Molecule 4 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	1766	Total	C	N	O	S	0	0
			11842	7410	2168	2213	51		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-1	SER	-	expression tag	UNP Q8N201
a	0	ASN	-	expression tag	UNP Q8N201

- Molecule 5 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	1051	Total	C	N	O	S	0	0
			8099	5198	1368	1471	62		

- Molecule 6 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	823	Total	C	N	O	S	0	0
			6443	4112	1099	1196	36		

- Molecule 7 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	873	Total	C	N	O	S	0	0
			6373	4050	1161	1135	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-1	SER	-	expression tag	UNP Q6P9B9
e	0	ASN	-	expression tag	UNP Q6P9B9

- Molecule 8 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	561	Total	C	N	O	S	0	0
			4422	2827	754	815	26		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-4	TYR	-	expression tag	UNP Q9UL03
f	-3	PHE	-	expression tag	UNP Q9UL03
f	-2	GLN	-	expression tag	UNP Q9UL03
f	-1	SER	-	expression tag	UNP Q9UL03
f	0	ASN	-	expression tag	UNP Q9UL03

- Molecule 9 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	889	Total	C	N	O	S	0	0
			6764	4283	1173	1267	41		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-1	SER	-	expression tag	UNP Q9NVH2
g	0	ASN	-	expression tag	UNP Q9NVH2

- Molecule 10 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	h	956	Total	C	N	O	S	0	0
			7623	4877	1297	1403	46		

- Molecule 11 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	626	Total	C	N	O	S	0	0
			4871	3137	792	909	33		

- Molecule 12 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	589	Total	C	N	O	S	0	0
			4411	2822	768	790	31		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	-1	SER	-	expression tag	UNP Q5TA45
k	0	ASN	-	expression tag	UNP Q5TA45
k	203	GLN	GLU	engineered mutation	UNP Q5TA45

- Molecule 13 is a protein called Integrator complex subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	m	542	Total	C	N	O	0	0
			2810	1682	568	560		

- Molecule 14 is a protein called Integrator complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	j	653	Total	C	N	O	0	0
			3238	1932	653	653		

- Molecule 15 is a protein called Integrator complex subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	n	503	Total	C	N	O	0	0
			2484	1478	503	503		

- Molecule 16 is a protein called Integrator complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	o	372	Total	C	N	O	0	0
			1849	1105	372	372		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	-1	SER	-	expression tag	UNP Q96N11
o	0	ASN	-	expression tag	UNP Q96N11

- Molecule 17 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	q	2	Total	Mn	0
			2	2	

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

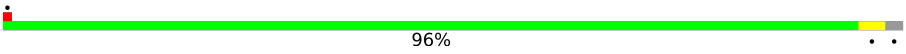
Mol	Chain	Residues	Atoms		AltConf
18	k	2	Total	Zn	0
			2	2	

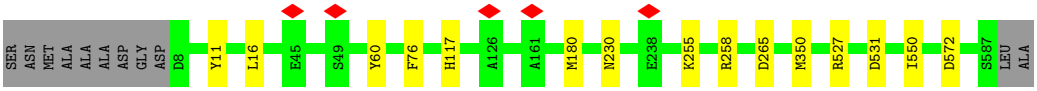
3 Residue-property plots (i)

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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

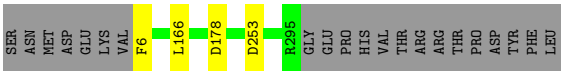
Chain p:





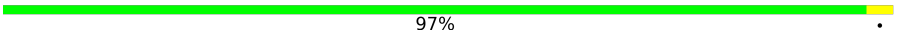
• Molecule 2: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain q:



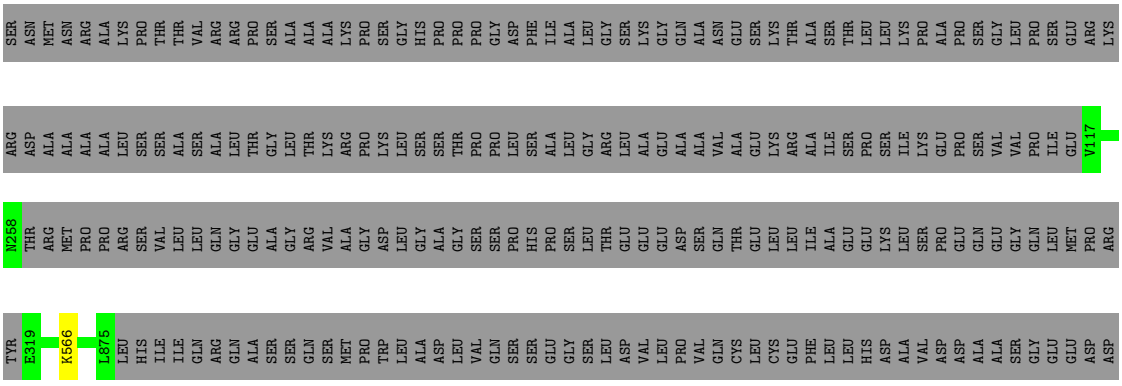
• Molecule 3: DSS1

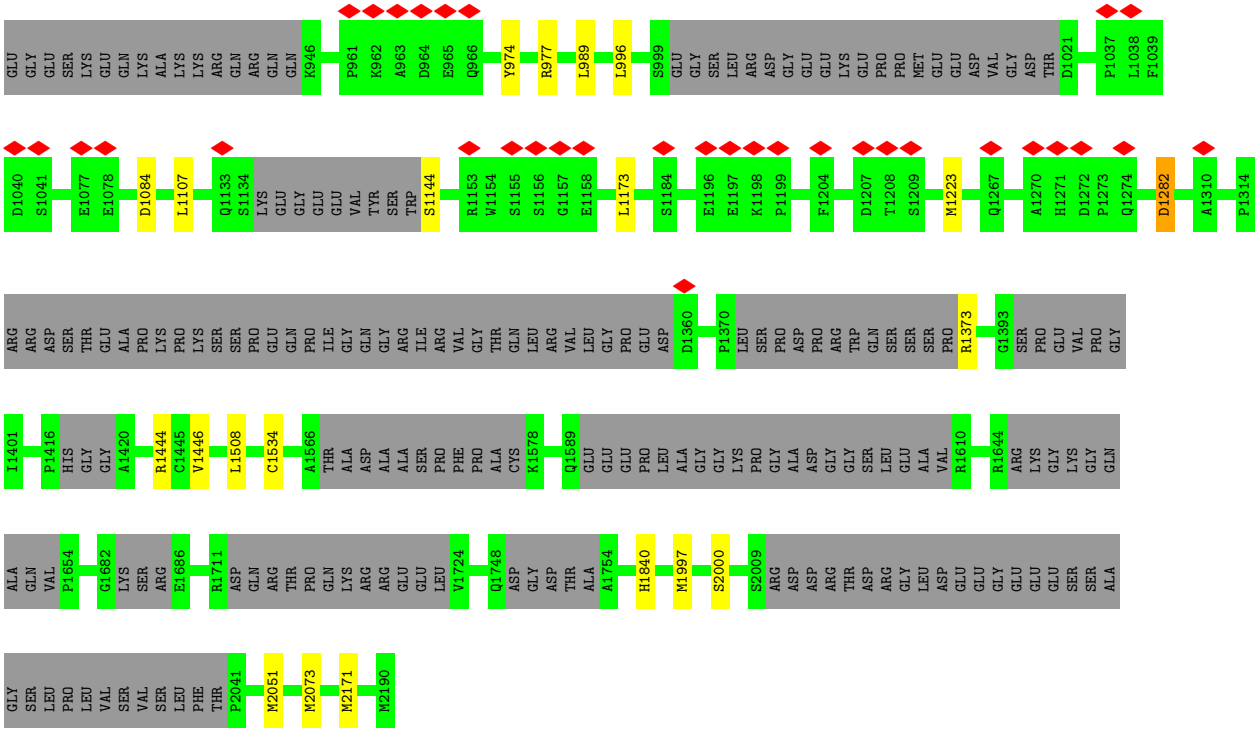
Chain r:



• Molecule 4: Integrator complex subunit 1

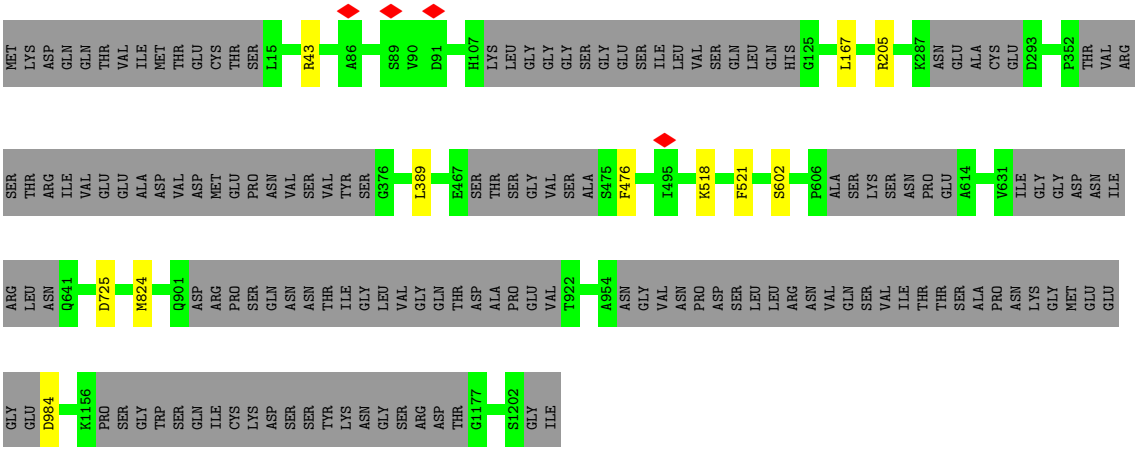
Chain a:





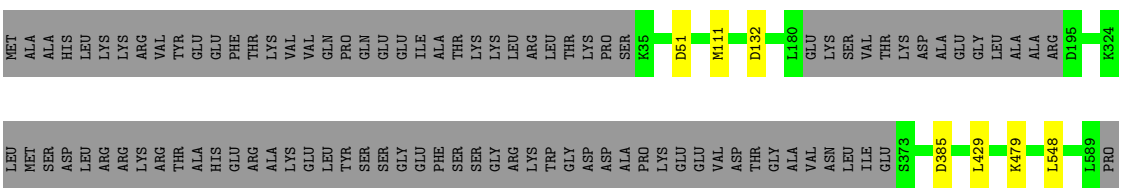
• Molecule 5: Integrator complex subunit 2

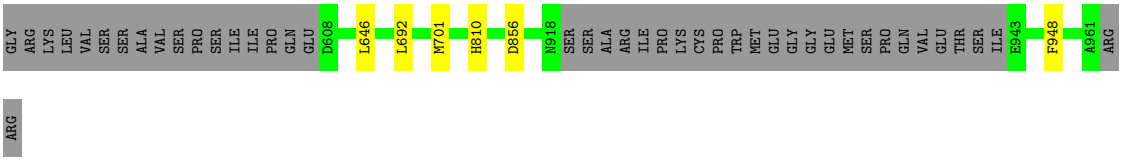
Chain b:



• Molecule 6: Integrator complex subunit 4

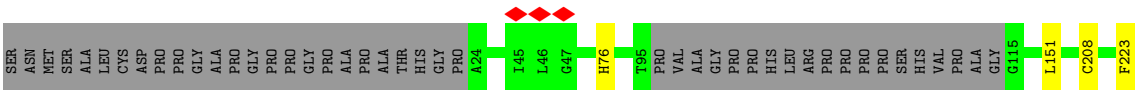
Chain d:

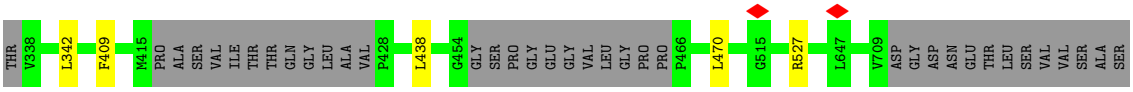


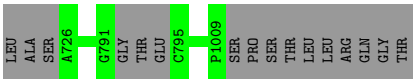


• Molecule 7: Integrator complex subunit 5

Chain e:

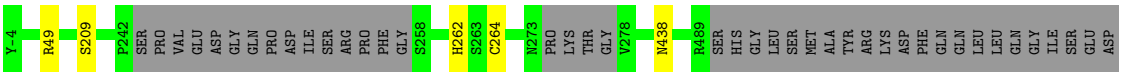






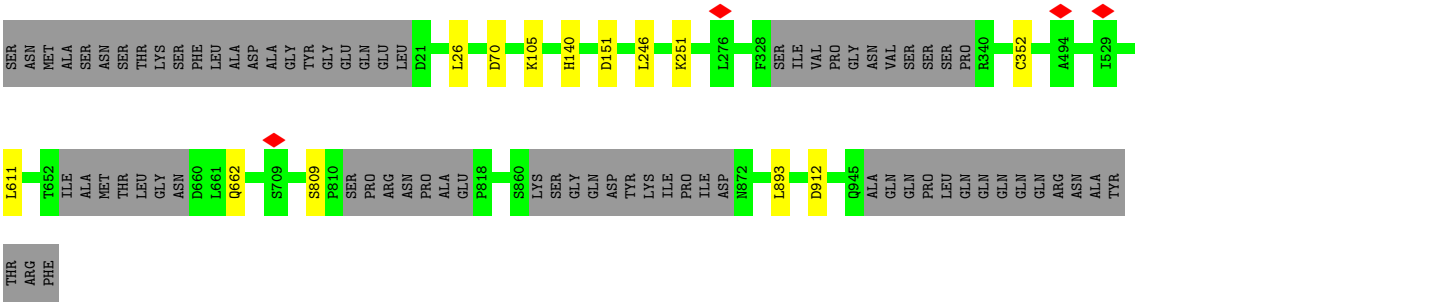
• Molecule 8: Integrator complex subunit 6

Chain f:



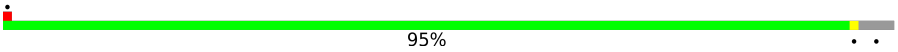
• Molecule 9: Integrator complex subunit 7

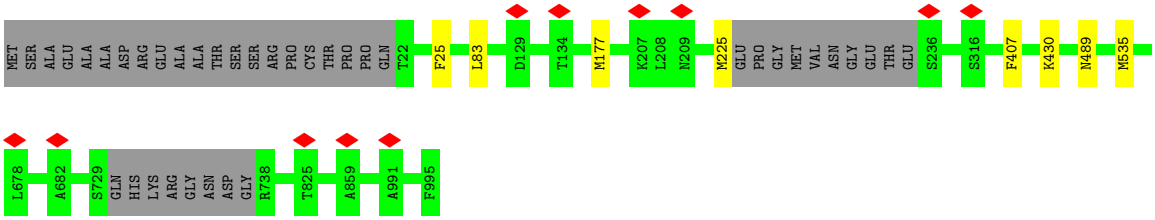
Chain g:



• Molecule 10: Integrator complex subunit 8

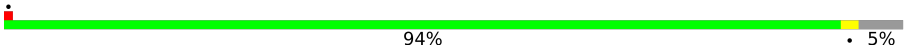
Chain h:

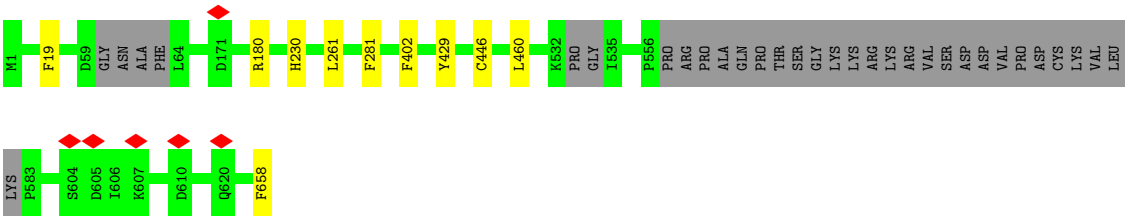




• Molecule 11: Integrator complex subunit 9

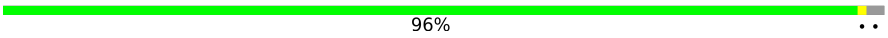
Chain i:





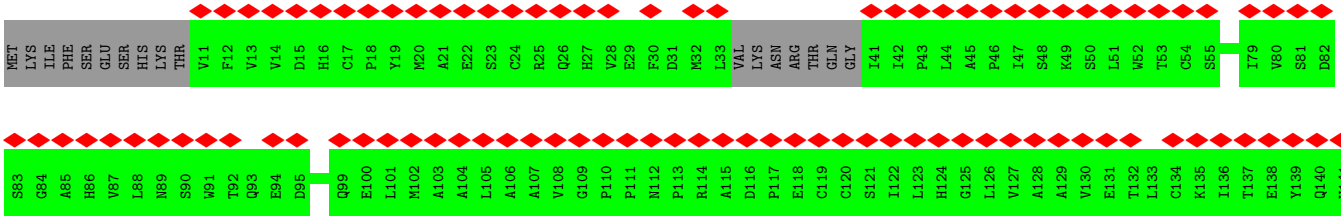
• Molecule 12: Integrator complex subunit 11

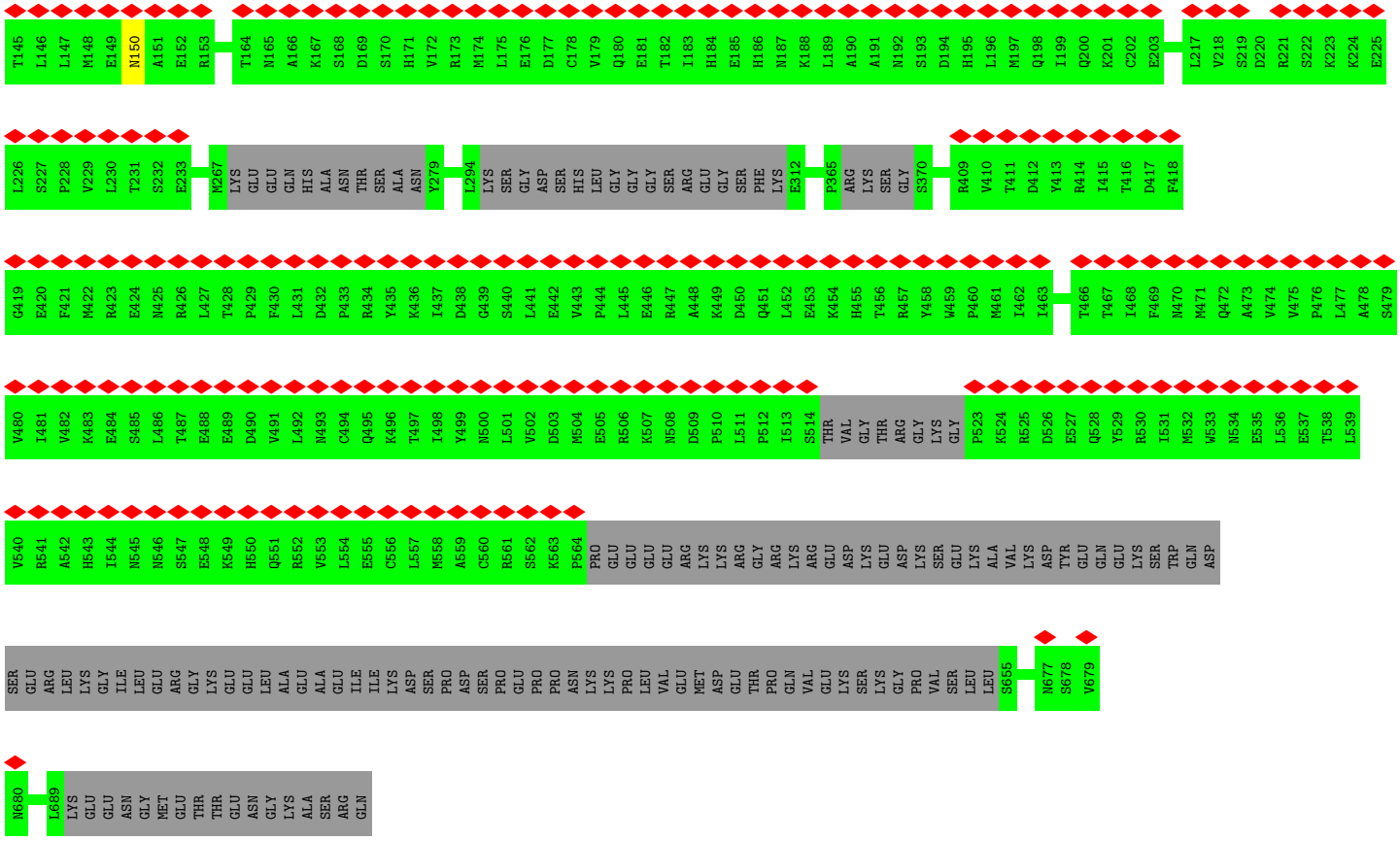
Chain k:



• Molecule 13: Integrator complex subunit 13

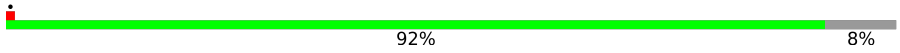
Chain m:

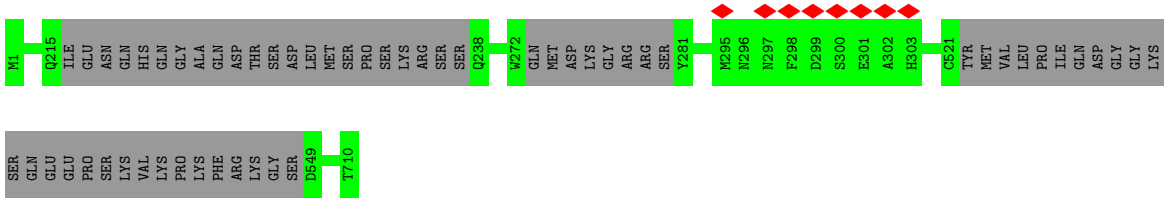




• Molecule 14: Integrator complex subunit 10

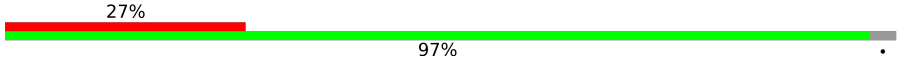
Chain j:

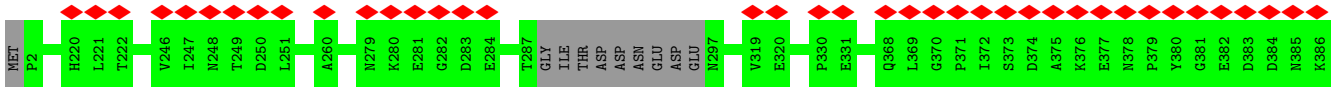


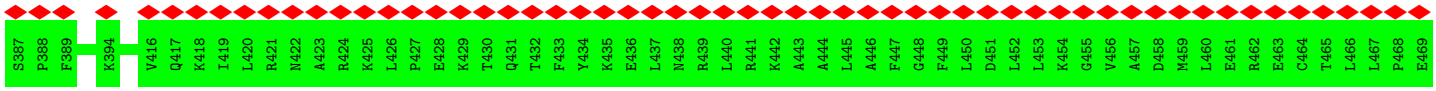


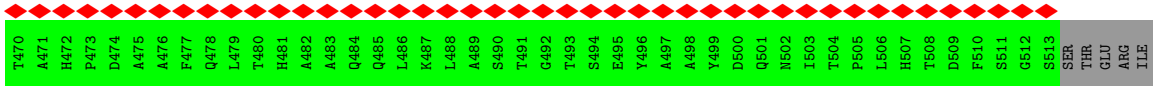
• Molecule 15: Integrator complex subunit 14

Chain n:



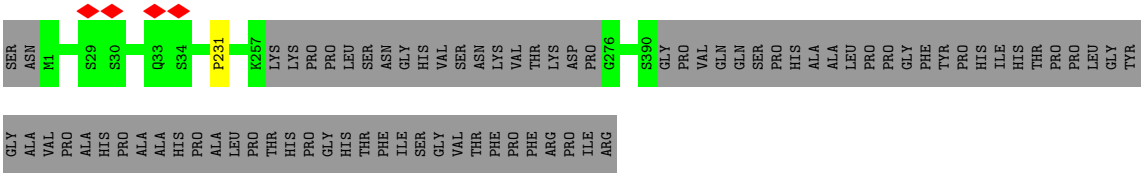






• Molecule 16: Integrator complex subunit 15

Chain o:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2335349	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.00502	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, MN

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	p	0.33	0/4511	0.56	2/6136 (0.0%)
2	q	0.41	0/2397	0.63	2/3250 (0.1%)
3	r	0.37	0/267	0.66	0/362
4	a	0.27	0/11994	0.55	6/16391 (0.0%)
5	b	0.31	0/8242	0.55	2/11212 (0.0%)
6	d	0.28	0/6568	0.57	5/8919 (0.1%)
7	e	0.32	0/6520	0.56	3/8895 (0.0%)
8	f	0.30	0/4531	0.56	1/6154 (0.0%)
9	g	0.29	0/6874	0.52	2/9324 (0.0%)
10	h	0.30	0/7768	0.51	0/10530
11	i	0.29	0/4990	0.56	0/6802
12	k	0.28	0/4508	0.58	0/6119
13	m	0.24	0/2809	0.47	0/3897
14	j	0.24	0/3234	0.38	0/4505
15	n	0.25	0/2482	0.46	0/3453
16	o	0.25	0/1847	0.40	0/2576
All	All	0.30	0/79542	0.54	23/108525 (0.0%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	q	253	ASP	CB-CG-OD2	10.07	127.36	118.30
4	a	1282	ASP	CB-CG-OD2	8.65	126.08	118.30
7	e	151	LEU	CA-CB-CG	7.66	132.91	115.30
7	e	438	LEU	CA-CB-CG	7.04	131.50	115.30
1	p	16	LEU	CA-CB-CG	6.70	130.70	115.30

There are no chirality outliers.

There are no planarity outliers.

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	p	4437	0	4508	0	0
2	q	2340	0	2248	0	0
3	r	263	0	229	0	0
4	a	11842	0	10065	0	0
5	b	8099	0	8211	0	0
6	d	6443	0	6483	0	0
7	e	6373	0	6187	0	0
8	f	4422	0	4393	0	0
9	g	6764	0	6747	0	0
10	h	7623	0	7779	0	0
11	i	4871	0	4849	0	0
12	k	4411	0	4248	0	0
13	m	2810	0	1353	0	0
14	j	3238	0	1433	0	0
15	n	2484	0	1104	0	0
16	o	1849	0	811	0	0
17	q	2	0	0	0	0
18	k	2	0	0	0	0
All	All	78273	0	70648	0	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 3.

There are no clashes within the asymmetric unit.

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	p	578/591 (98%)	567 (98%)	11 (2%)	0	100	100
2	q	288/311 (93%)	273 (95%)	15 (5%)	0	100	100
3	r	29/31 (94%)	29 (100%)	0	0	100	100
4	a	1734/2192 (79%)	1682 (97%)	51 (3%)	1 (0%)	51	83
5	b	1031/1204 (86%)	983 (95%)	48 (5%)	0	100	100
6	d	813/963 (84%)	791 (97%)	22 (3%)	0	100	100
7	e	857/1021 (84%)	824 (96%)	33 (4%)	0	100	100
8	f	551/892 (62%)	535 (97%)	16 (3%)	0	100	100
9	g	879/964 (91%)	847 (96%)	32 (4%)	0	100	100
10	h	950/995 (96%)	927 (98%)	23 (2%)	0	100	100
11	i	618/658 (94%)	588 (95%)	30 (5%)	0	100	100
12	k	583/602 (97%)	540 (93%)	42 (7%)	1 (0%)	47	79
13	m	528/706 (75%)	491 (93%)	36 (7%)	1 (0%)	47	79
14	j	645/710 (91%)	626 (97%)	19 (3%)	0	100	100
15	n	499/518 (96%)	466 (93%)	33 (7%)	0	100	100
16	o	368/451 (82%)	347 (94%)	20 (5%)	1 (0%)	41	73
All	All	10951/12809 (86%)	10516 (96%)	431 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	k	310	ARG
16	o	231	PRO
4	a	566	LYS
13	m	150	ASN

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	p	487/514 (95%)	474 (97%)	13 (3%)	44	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	q	255/276 (92%)	253 (99%)	2 (1%)	81 92
3	r	28/28 (100%)	27 (96%)	1 (4%)	35 67
4	a	931/1909 (49%)	915 (98%)	16 (2%)	60 83
5	b	894/1072 (83%)	885 (99%)	9 (1%)	76 90
6	d	709/845 (84%)	700 (99%)	9 (1%)	69 87
7	e	630/814 (77%)	621 (99%)	9 (1%)	67 86
8	f	491/801 (61%)	482 (98%)	9 (2%)	59 82
9	g	733/842 (87%)	722 (98%)	11 (2%)	65 85
10	h	859/896 (96%)	851 (99%)	8 (1%)	78 91
11	i	555/600 (92%)	545 (98%)	10 (2%)	59 82
12	k	443/522 (85%)	435 (98%)	8 (2%)	59 82
13	m	31/639 (5%)	31 (100%)	0	100 100
All	All	7046/9758 (72%)	6941 (98%)	105 (2%)	66 85

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	e	409	PHE
9	g	140	HIS
12	k	87	ASP
8	f	49	ARG
8	f	561	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	p	479	HIS
1	p	520	HIS
10	h	170	GLN
11	i	389	GLN
11	i	418	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 4 ligands modelled in this entry, 4 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.

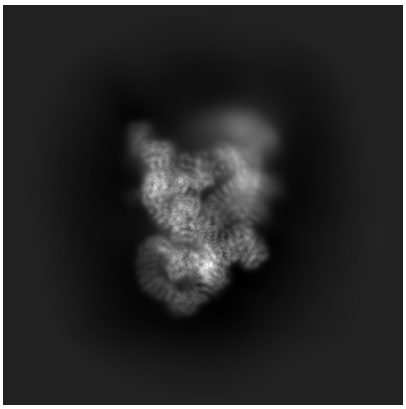
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19047. These allow visual inspection of the internal detail of the map and identification of artifacts.

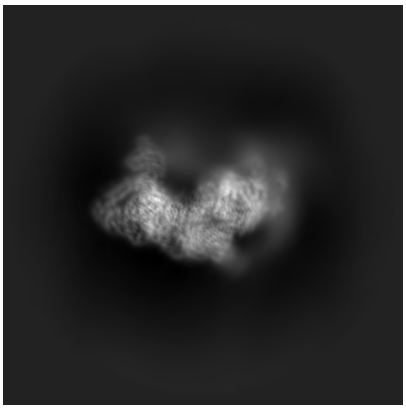
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

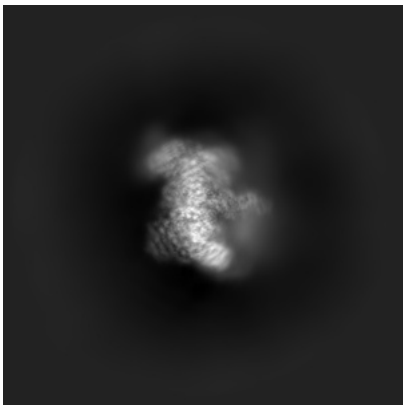
6.1.1 Primary map



X

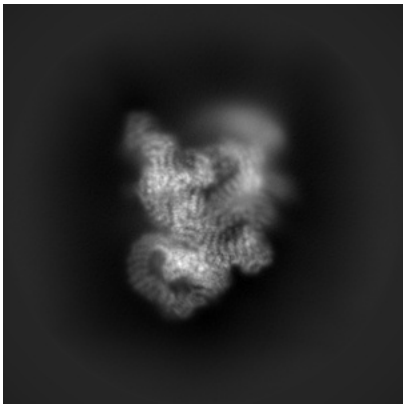


Y

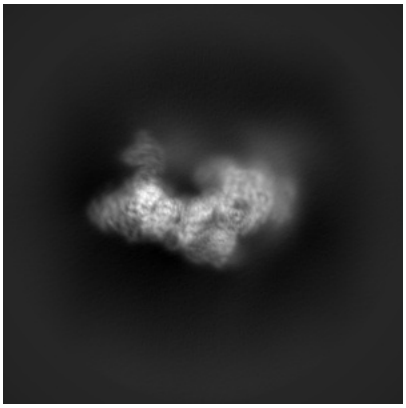


Z

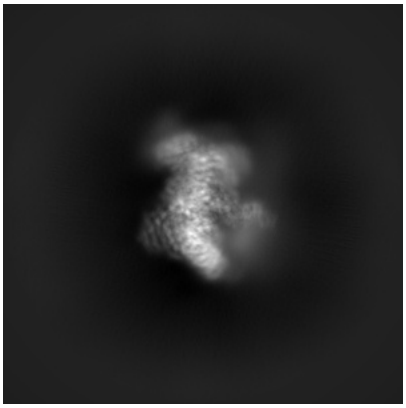
6.1.2 Raw map



X



Y

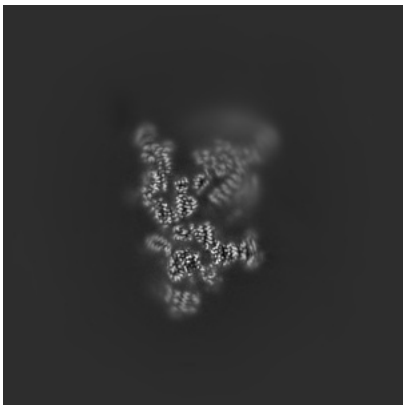


Z

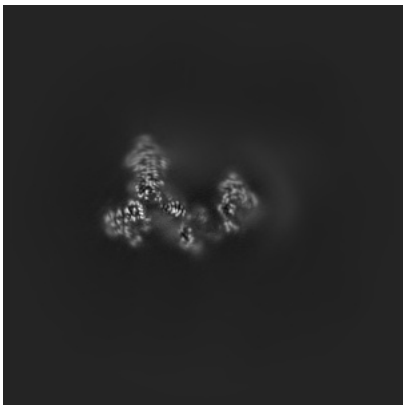
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

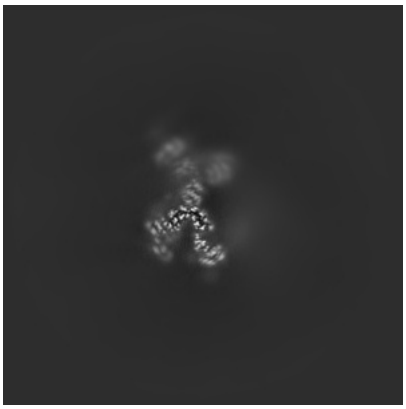
6.2.1 Primary map



X Index: 240

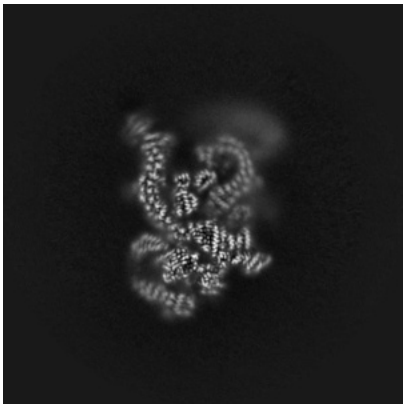


Y Index: 240

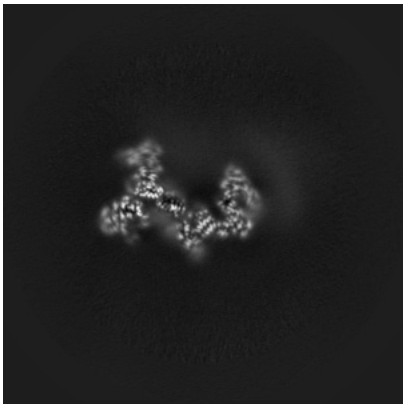


Z Index: 240

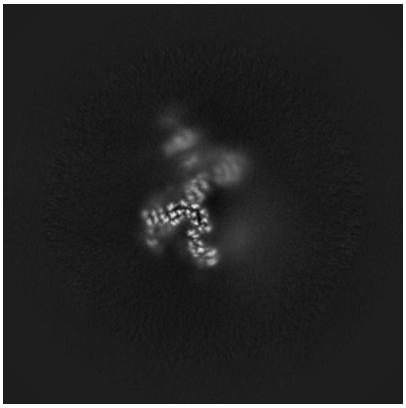
6.2.2 Raw map



X Index: 240



Y Index: 240

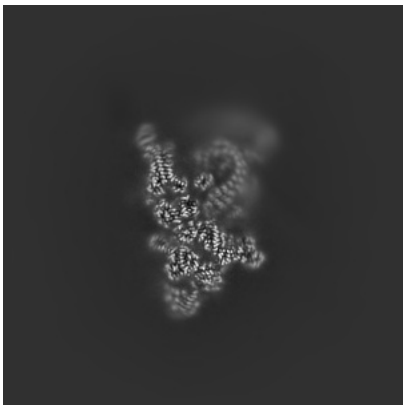


Z Index: 240

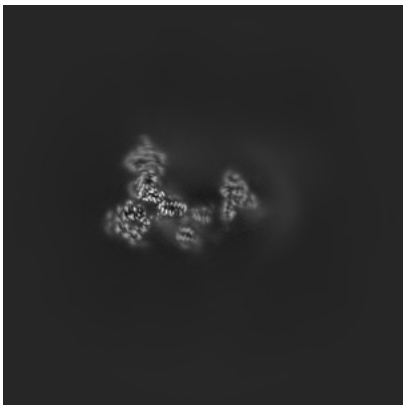
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

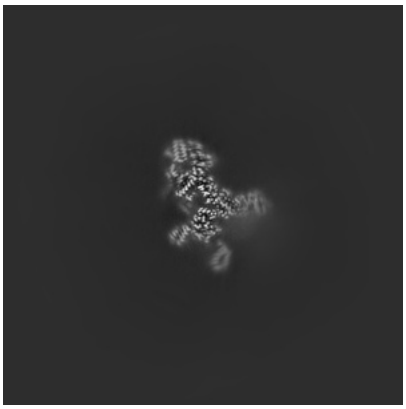
6.3.1 Primary map



X Index: 235

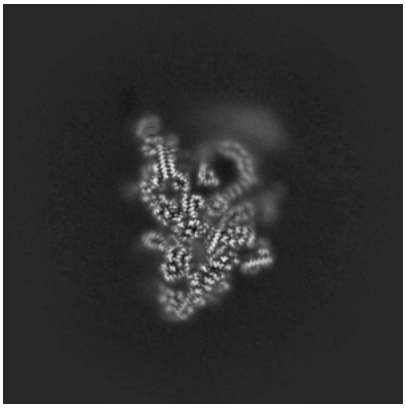


Y Index: 245

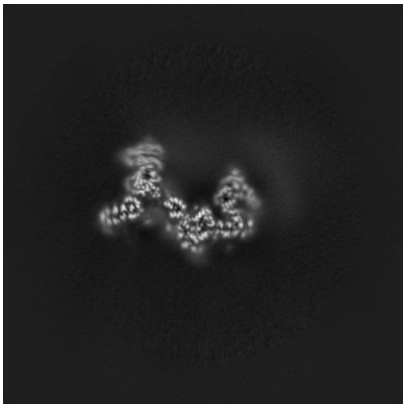


Z Index: 177

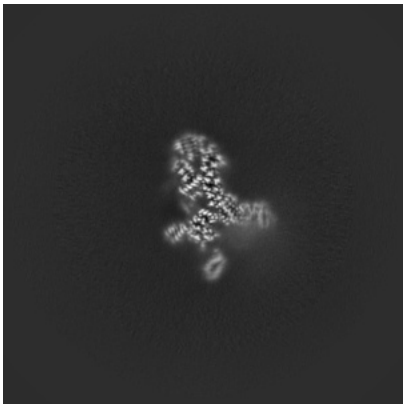
6.3.2 Raw map



X Index: 230



Y Index: 236

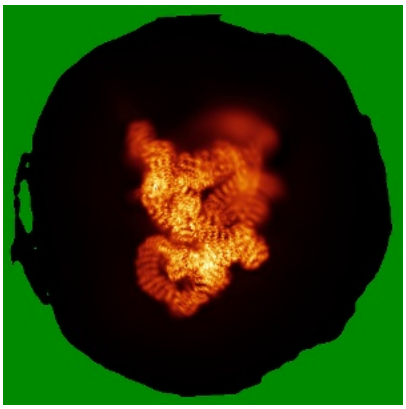


Z Index: 175

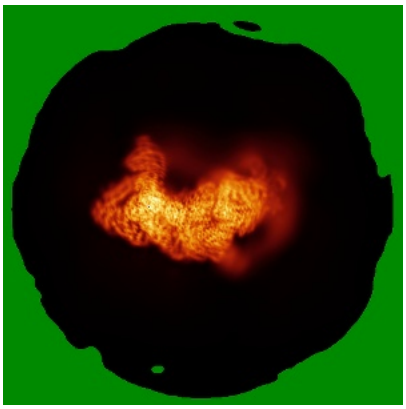
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

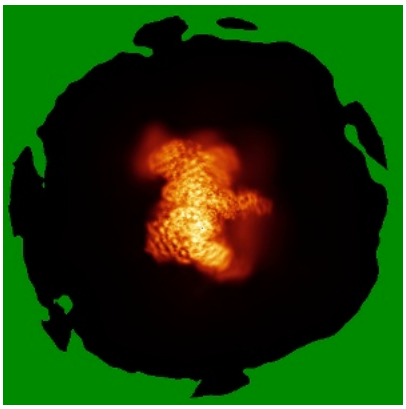
6.4.1 Primary map



X

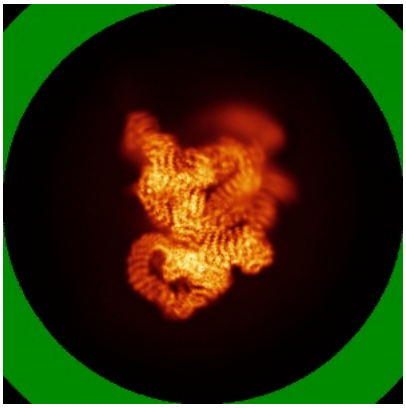


Y

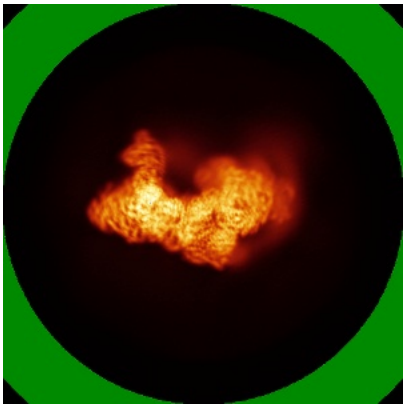


Z

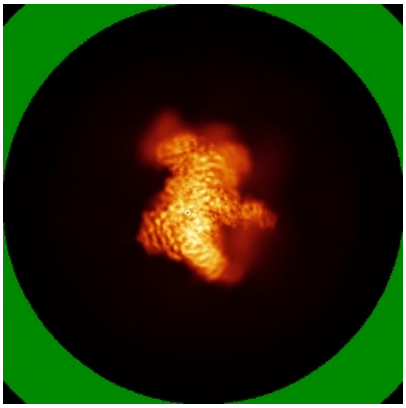
6.4.2 Raw map



X



Y

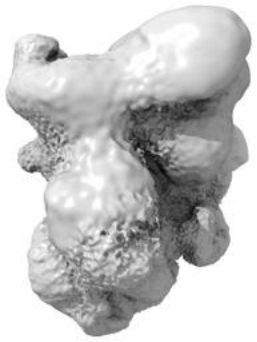


Z

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.

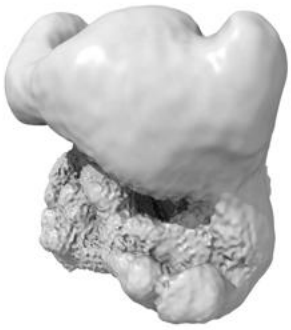
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

Y

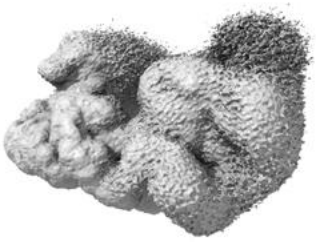


Z

The images above show the 3D surface view of the map at the recommended contour level 0.00502. 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

X



Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

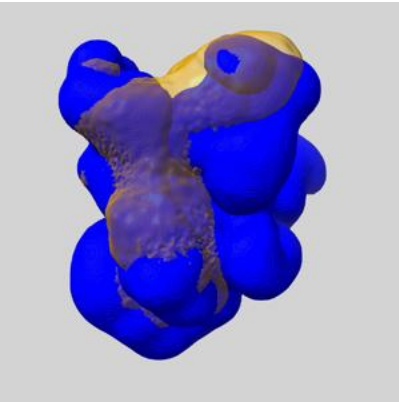
6.6 Mask visualisation (i)

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

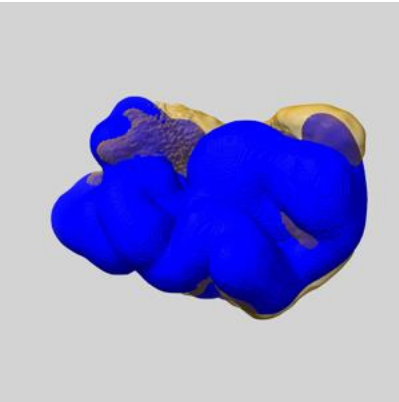
A mask typically either:

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

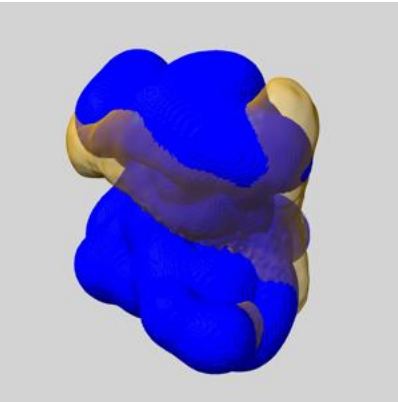
6.6.1 emd_19047_msk_1.map (i)



X



Y

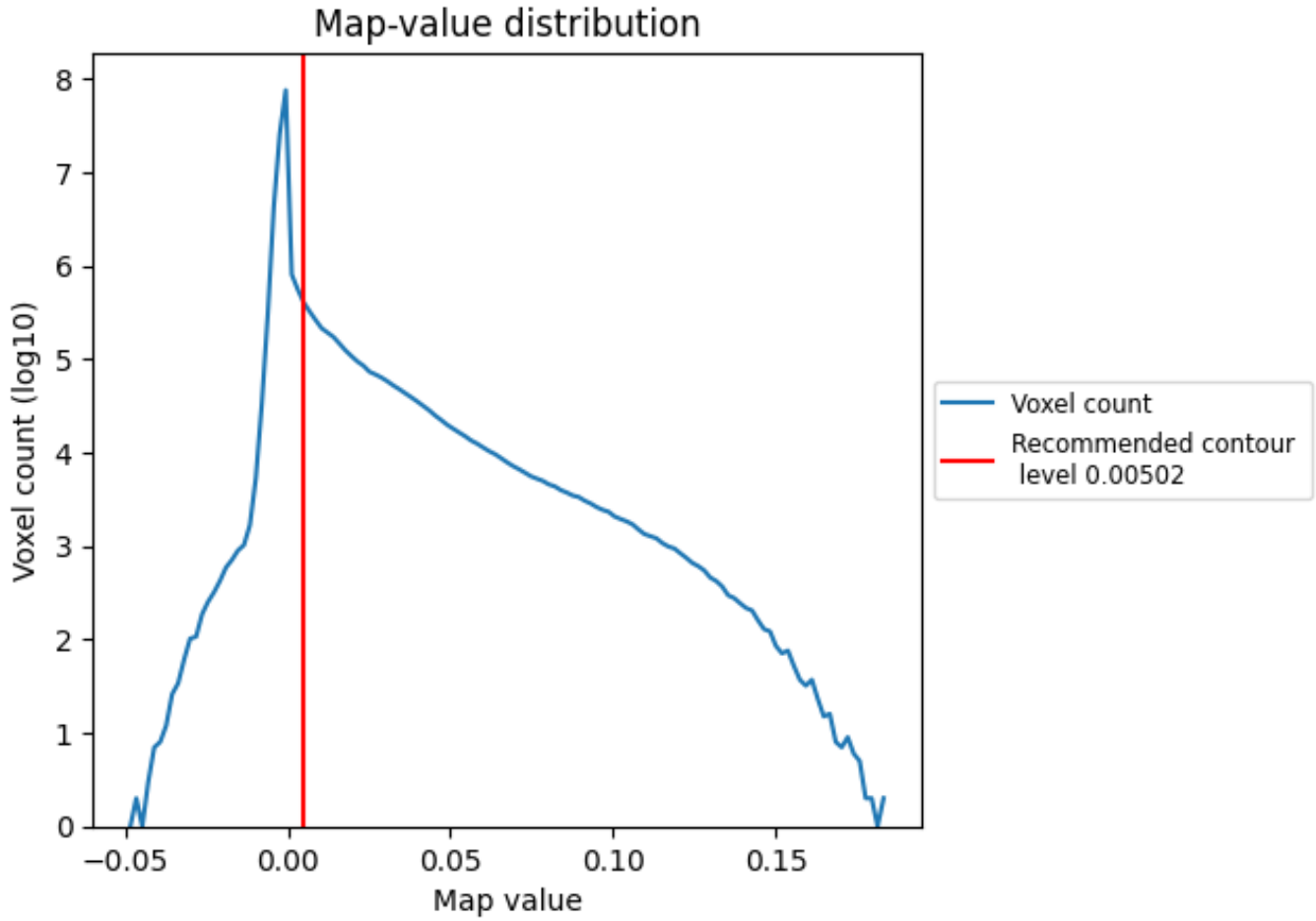


Z

7 Map analysis

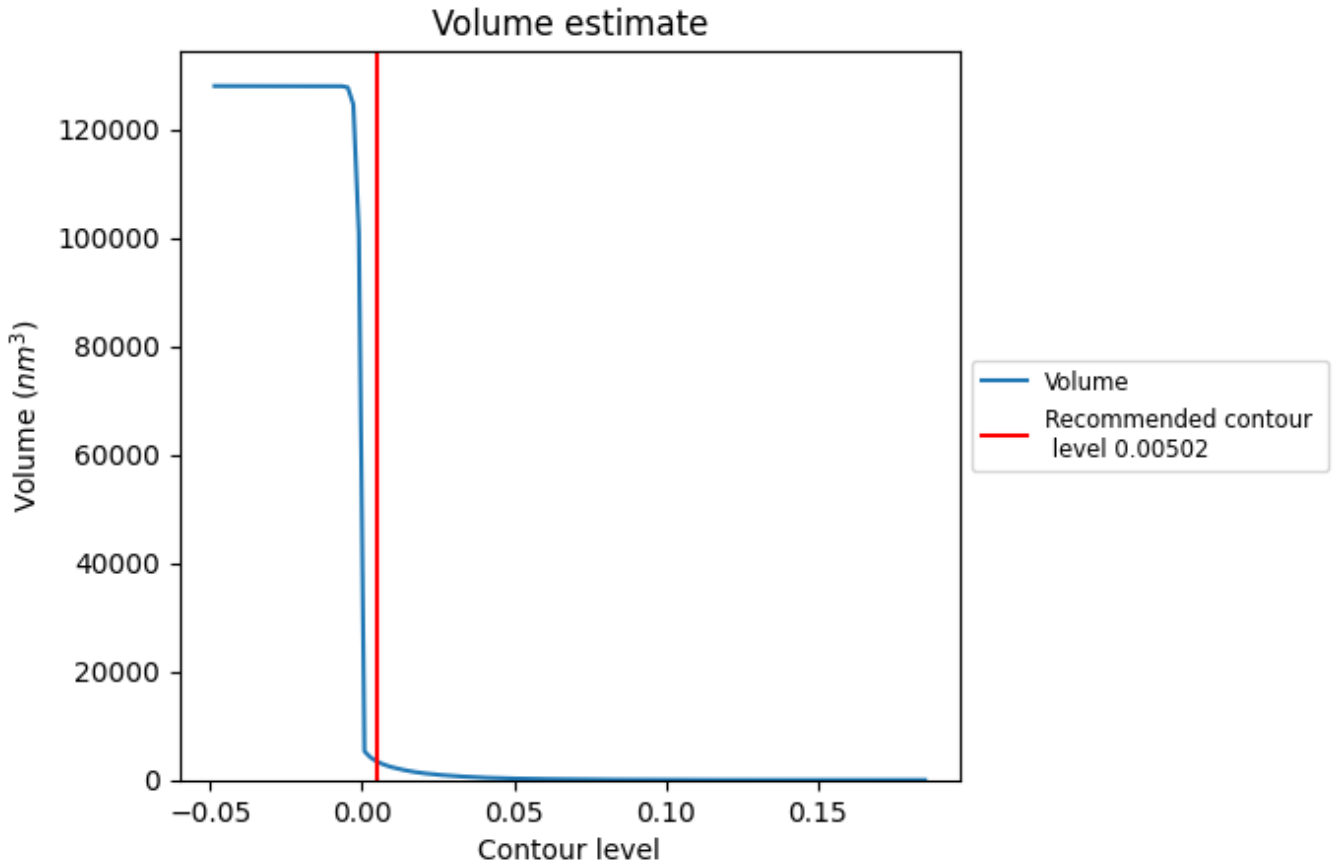
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

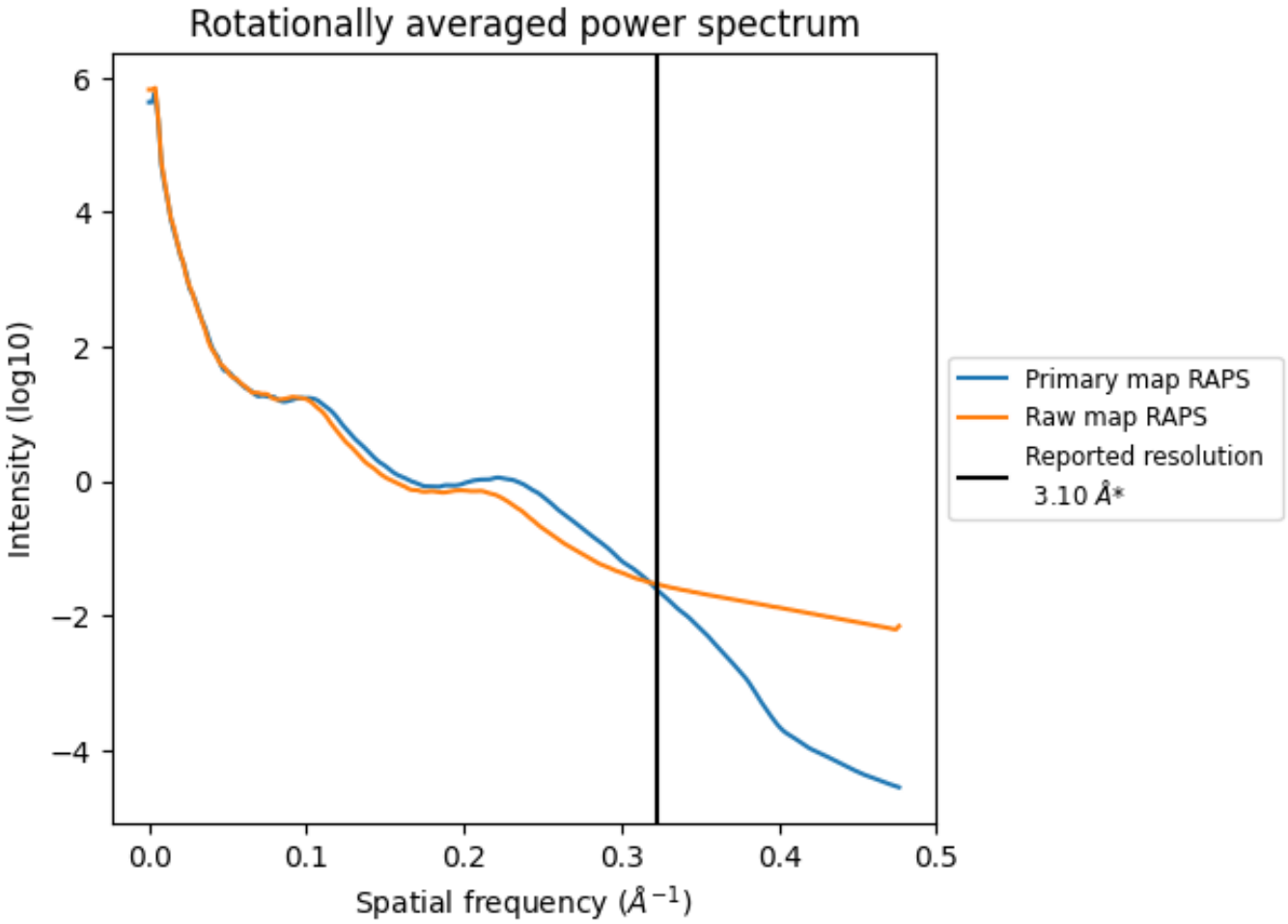
7.2 Volume estimate (i)



The volume at the recommended contour level is 3389 nm^3; this corresponds to an approximate mass of 3061 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)

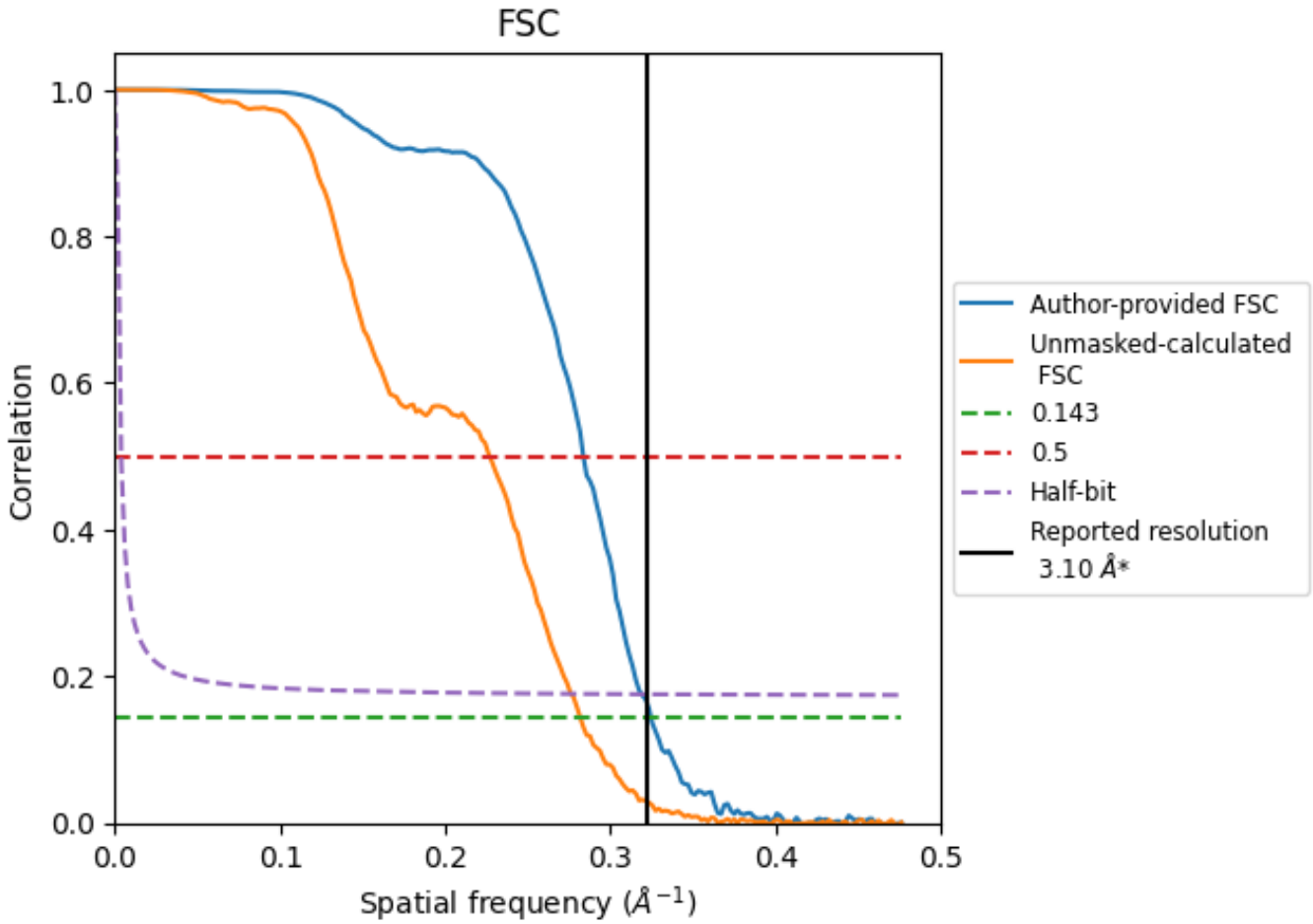


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

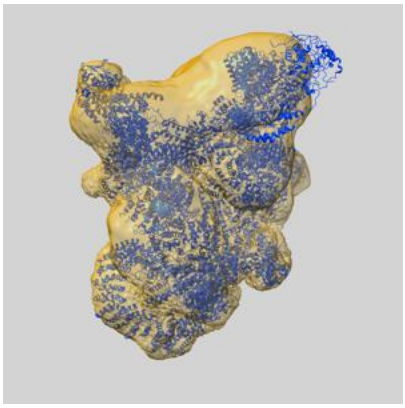
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.52	3.13
Unmasked-calculated*	3.55	4.41	3.62

*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 3.55 differs from the reported value 3.1 by more than 10 %

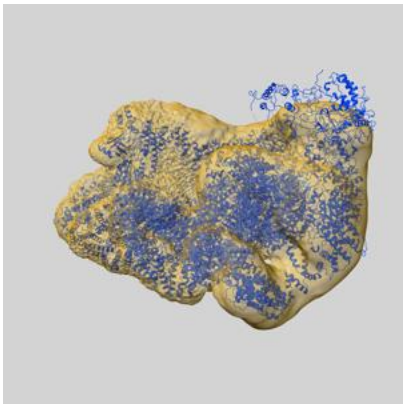
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19047 and PDB model 8RC4. Per-residue inclusion information can be found in section 3 on page 8.

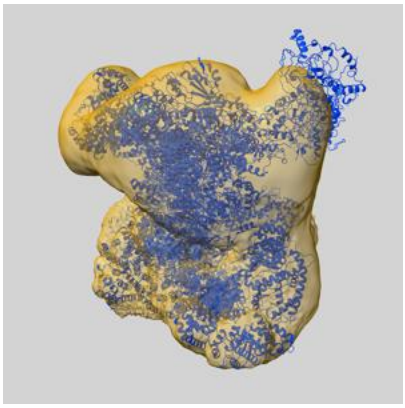
9.1 Map-model overlay



X



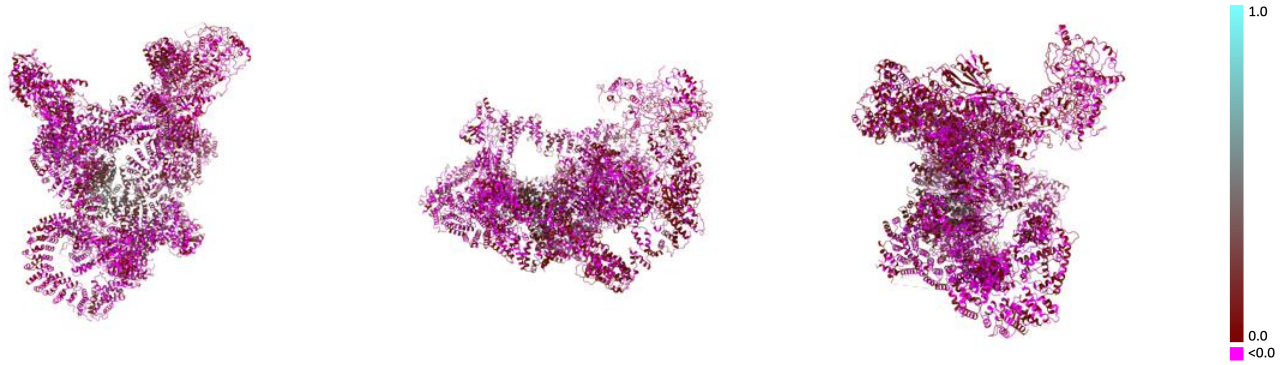
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00502 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.

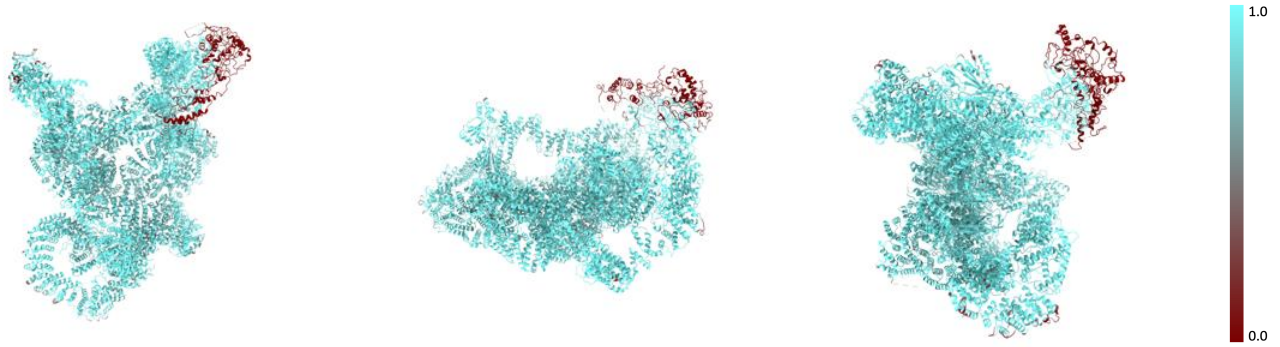
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

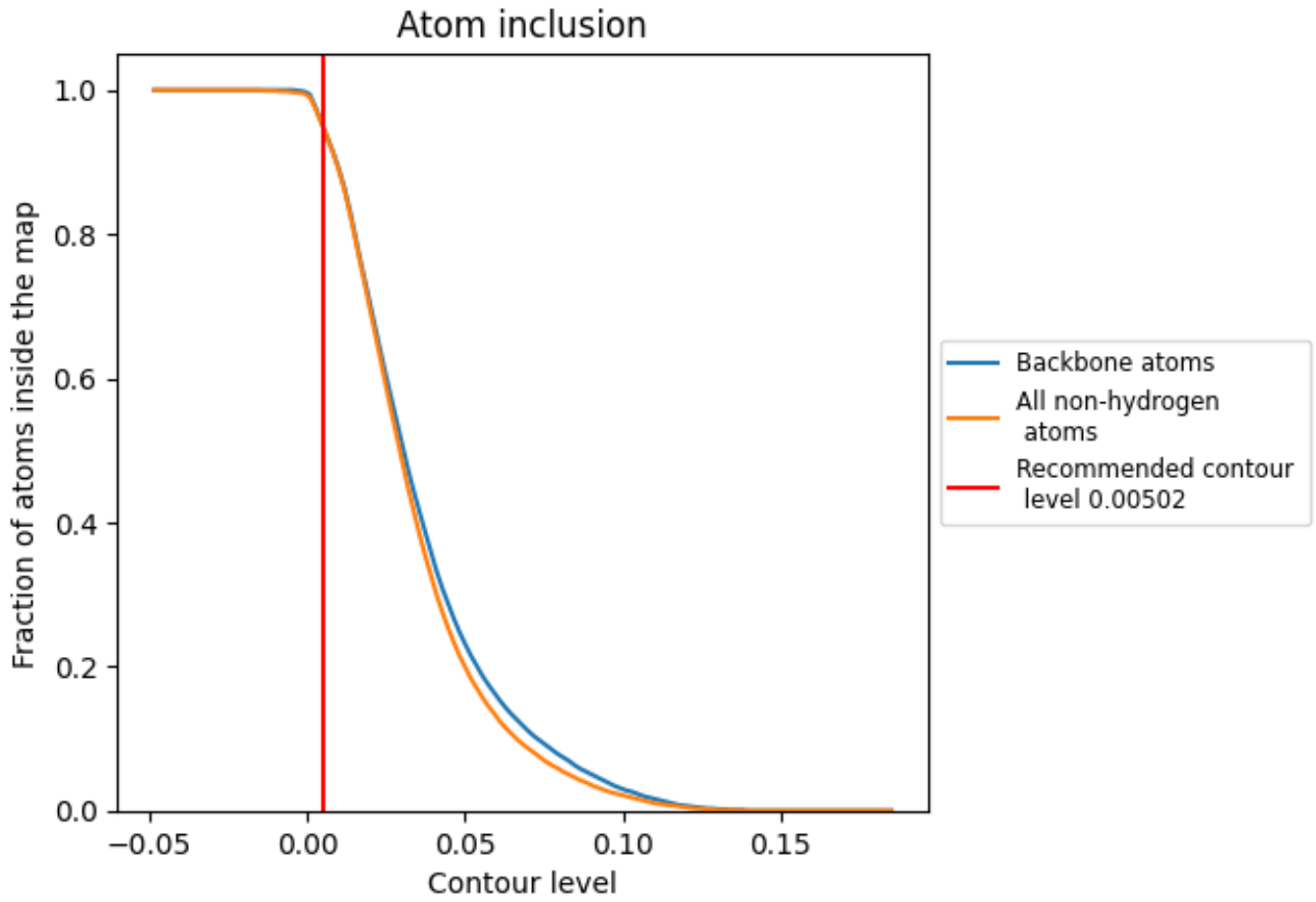
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.00502).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.00502) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9490	0.0360
a	0.9690	0.0540
b	0.9790	0.0870
d	0.9900	0.0350
e	0.9700	0.0110
f	0.9870	0.0240
g	0.9670	0.0460
h	0.9630	0.0100
i	0.9840	0.0020
j	0.9860	0.0510
k	0.9990	0.0440
m	0.4430	0.0190
n	0.7180	0.0230
o	0.9890	0.0540
p	0.9760	0.0390
q	0.9660	-0.0370
r	0.9530	-0.0080