



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 03:09 AM UTC

PDB ID : 9PGH / pdb_00009pgh
EMDB ID : EMD-71632
Title : The cryo-EM structure of C. crescentus RNAP-Sigma73-CCNA_03891/CCNA_01149 promoter complex
Authors : Singh, R.R.; Schumacher, M.A.
Deposited on : 2025-07-07
Resolution : 3.54 Å(reported)
Based on initial model : 7ye1

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:

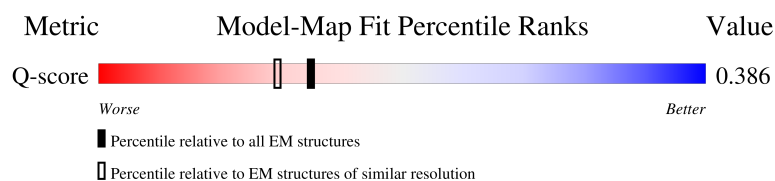
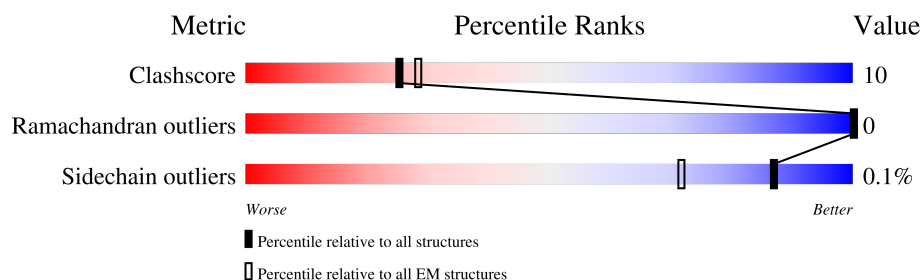
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.54 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.



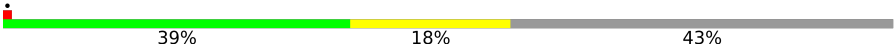

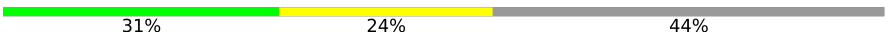

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12891 (3.04 - 4.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	 51% 18% 31%
1	B	338	 51% 20% 28%
2	C	1356	 77% 23% .
3	D	1396	 75% 21% .

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Mol	Chain	Length	Quality of chain
4	E	119	
5	F	652	
6	H	99	
7	I	99	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 30040 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	233	Total	C	N	O	S	0	0
			1763	1104	318	337	4		
1	B	243	Total	C	N	O	S	0	0
			1818	1141	328	345	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1349	Total	C	N	O	S	0	0
			10229	6445	1811	1932	41		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1339	Total	C	N	O	S	0	0
			10070	6345	1801	1880	44		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	68	Total	C	N	O	S	0	0
			508	313	93	100	2		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	486	Total	C	N	O	S	0	0
			3667	2300	663	692	12		

- Molecule 6 is a DNA chain called DNA (55-MER)-non template.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	55	Total	C	N	O	P	0	0
			1115	530	199	331	55		

- Molecule 7 is a DNA chain called DNA (43-MER)-template.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	42	Total	C	N	O	P	0	0
			867	408	165	252	42		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

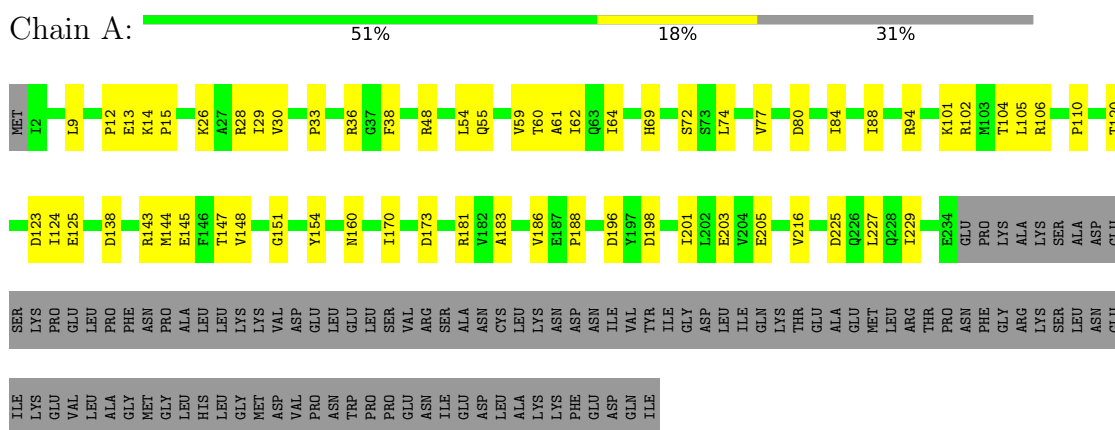
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

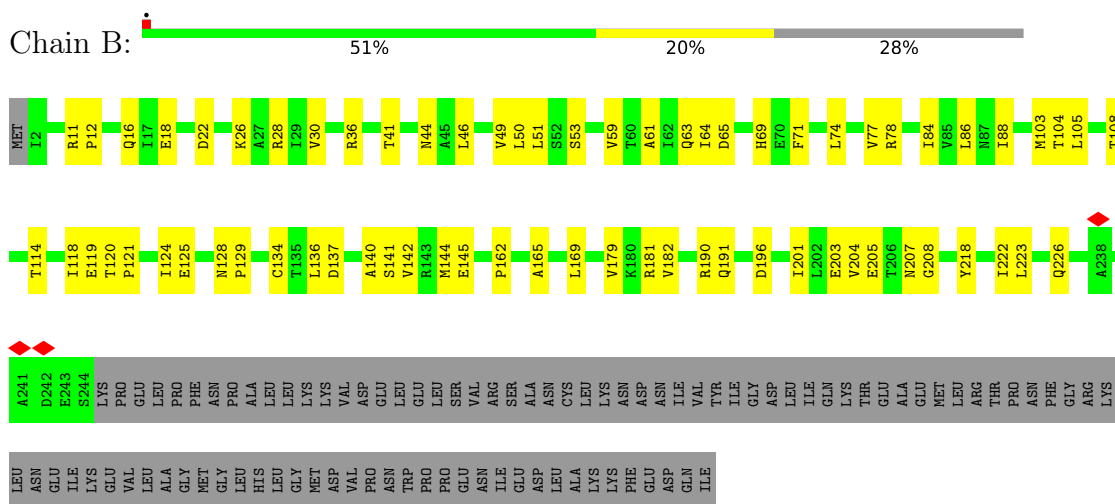
3 Residue-property plots

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.

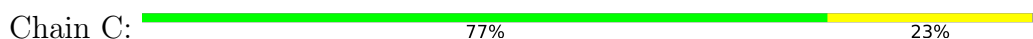
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

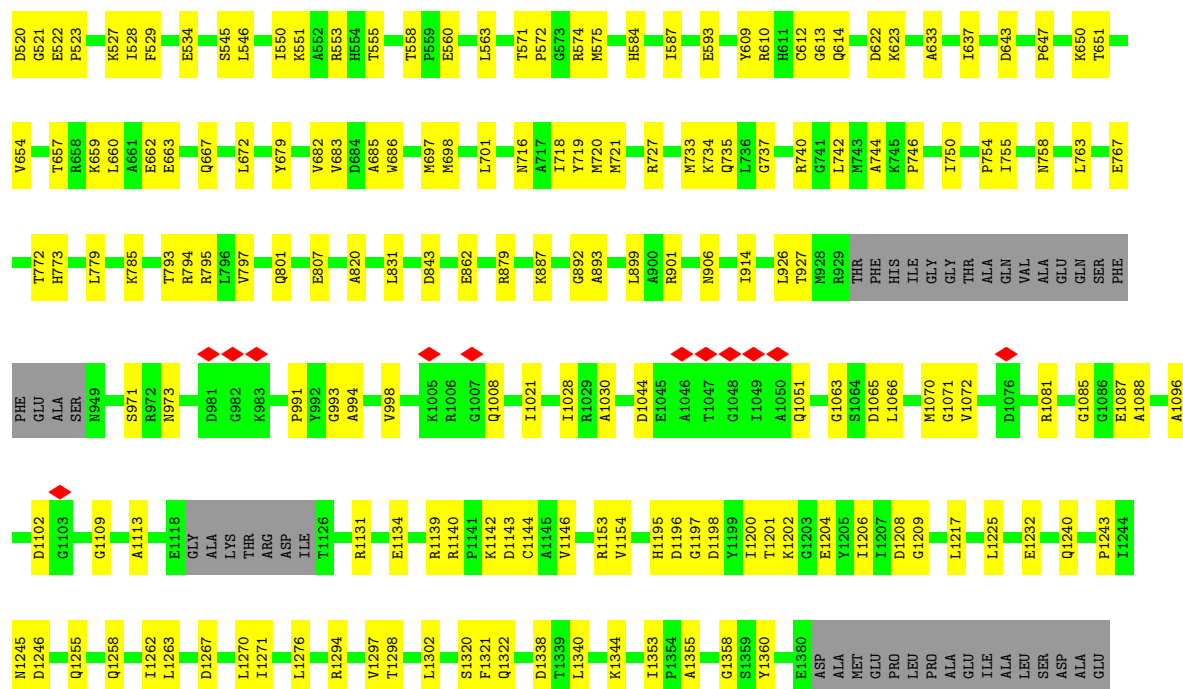


- Molecule 2: DNA-directed RNA polymerase subunit beta

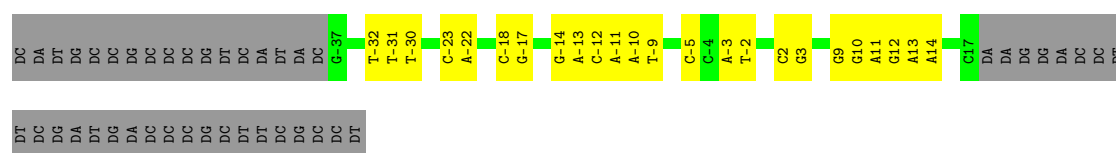
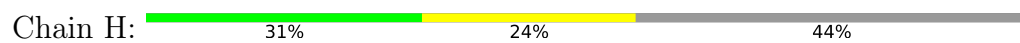




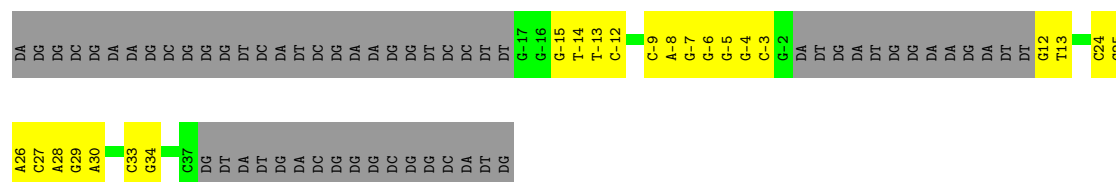
Q398	L254	M103	MET
R401	G259	M104	ASN
Q407	D269	H105	GLN
P408	L270	I106	GLU
Q409	T271	E107	VAL
W410	R272	L108	LEU
W411	G277	A109	ASN
	N276	K119	ILE
L414	R277		PHE
	L281	L121	ASN
W417	L285	P122	PRO
L418		S123	VAL
W426	L286	R124	GLM
A428	P290	M131	ALA
P429	T294	P132	ALA
	S304	L133	P16
Q436		K134	Q20
Q437	S308	I136	I21
A438	F309	R138	P28
	D310	V139	E29
Q436		L140	K30
A461	R313	Y141	I31
D462	T319	V145	R32
F463	L326	I146	S33
D464	K327	H158	S35
G465	L329	I152	E38
Q467	L329		I39
W468	M332	L190	K40
L474	K336	R204	R41
	R341	L207	P42
E477	L345	L223	I45
L480	D350	E227	R54
W487	L357	R235	D56
A488	P361	W238	R61
T489	E362	L241	K67
L493	L363	T242	E70
W497	H366	V243	C71
G498	S376	V244	L72
	L376	P245	K77
I501	L383	I247	Y81
P504	T395	P248	I84
S505	V396	L251	C89
O506	G397		G90
P507			L95
I508			V98
W509			
L510			



- Molecule 6: DNA (55-MER)-non template



- Molecule 7: DNA (43-MER)-template



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150644	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 ($e^-/\text{\AA}^2$)	58.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0033	Depositor
Map size (Å)	414.72003, 414.72003, 414.72003	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/1790	0.37	0/2438
1	B	0.15	0/1847	0.34	0/2519
2	C	0.15	0/10404	0.35	0/14097
3	D	0.16	0/10225	0.39	1/13825 (0.0%)
4	E	0.14	0/512	0.32	0/694
5	F	0.11	0/3708	0.30	0/5004
6	H	0.16	0/1247	0.32	0/1919
7	I	0.18	0/972	0.35	0/1497
All	All	0.15	0/30705	0.36	1/41993 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	361	PRO	CA-N-CD	-12.87	93.98	112.00

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	A	1763	0	1769	48	0
1	B	1818	0	1812	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10229	0	10044	222	0
3	D	10070	0	10051	216	0
4	E	508	0	505	14	0
5	F	3667	0	3594	73	0
6	H	1115	0	618	22	0
7	I	867	0	471	16	0
8	D	1	0	0	0	0
9	D	2	0	0	0	0
All	All	30040	0	28864	613	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 10.

The worst 5 of 613 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)
1:B:63:GLN:HB2	1:B:145:GLU:HB2	1.55	0.88
2:C:568:PRO:HB2	3:D:772:THR:HG21	1.58	0.85
1:A:64:ILE:HG22	1:A:144:MET:HG2	1.58	0.84
2:C:236:PHE:O	2:C:340:THR:HA	1.78	0.82
5:F:358:VAL:HA	5:F:361:MET:HE2	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/338 (68%)	211 (91%)	20 (9%)	0	100	100
1	B	241/338 (71%)	222 (92%)	19 (8%)	0	100	100
2	C	1345/1356 (99%)	1241 (92%)	104 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1333/1396 (96%)	1235 (93%)	98 (7%)	0	100	100
4	E	66/119 (56%)	63 (96%)	3 (4%)	0	100	100
5	F	480/652 (74%)	456 (95%)	24 (5%)	0	100	100
All	All	3696/4199 (88%)	3428 (93%)	268 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/285 (65%)	185 (100%)	0	100	100
1	B	187/285 (66%)	187 (100%)	0	100	100
2	C	1048/1137 (92%)	1048 (100%)	0	100	100
3	D	1028/1157 (89%)	1028 (100%)	0	100	100
4	E	54/100 (54%)	54 (100%)	0	100	100
5	F	364/542 (67%)	362 (100%)	2 (0%)	81	81
All	All	2866/3506 (82%)	2864 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	398	ARG
5	F	448	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	801	GLN
3	D	1334	HIS
5	F	576	GLN

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Mol	Chain	Res	Type
5	F	264	GLN
3	D	1248	HIS

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](#)

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.

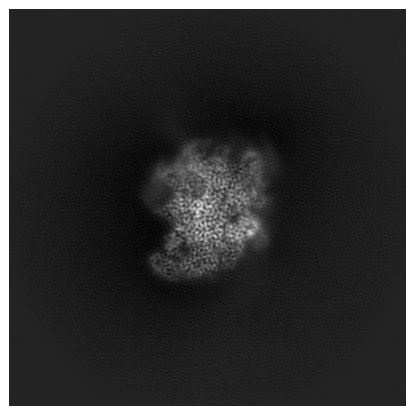
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71632. These allow visual inspection of the internal detail of the map and identification of artifacts.

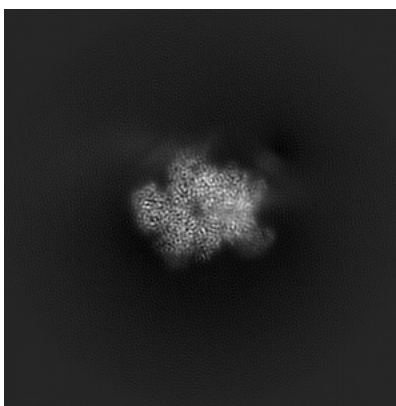
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

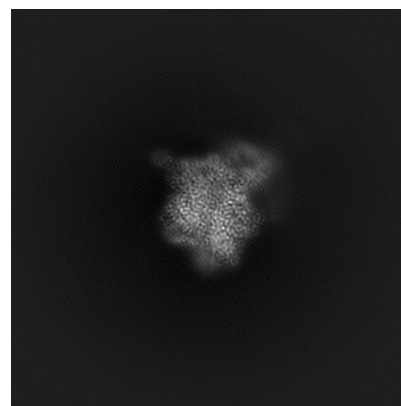
6.1.1 Primary map



X

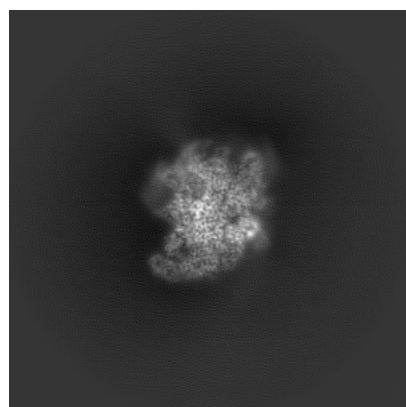


Y

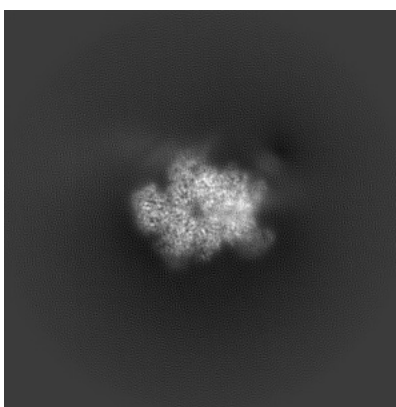


Z

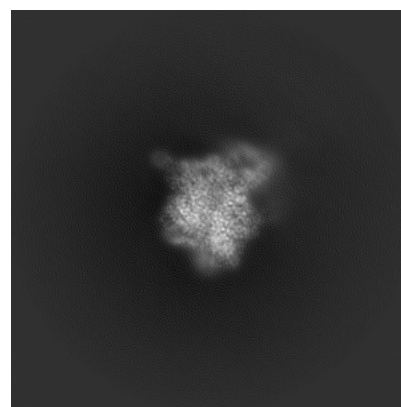
6.1.2 Raw map



X



Y

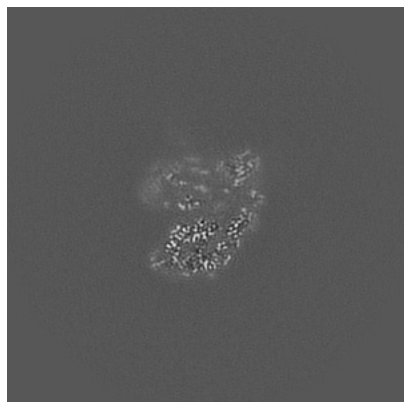


Z

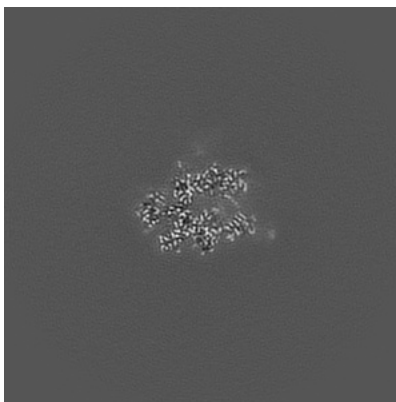
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

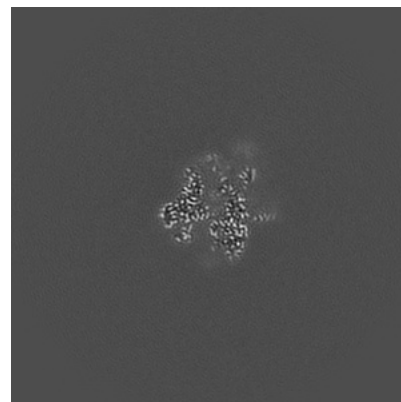
6.2.1 Primary map



X Index: 192

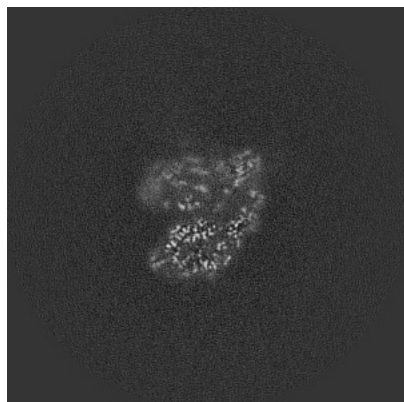


Y Index: 192

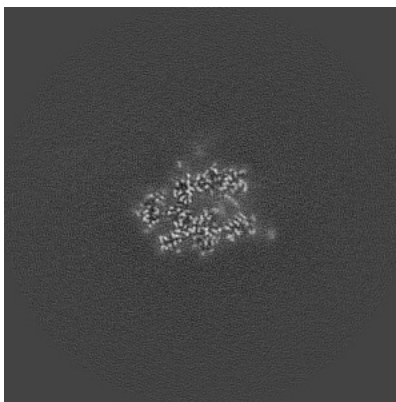


Z Index: 192

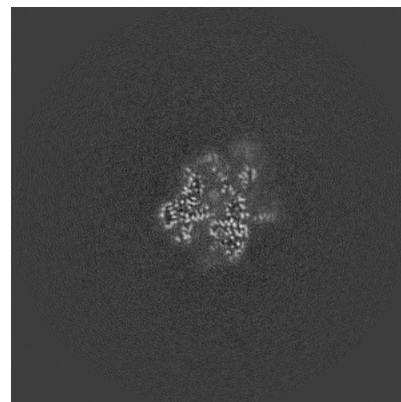
6.2.2 Raw map



X Index: 192



Y Index: 192

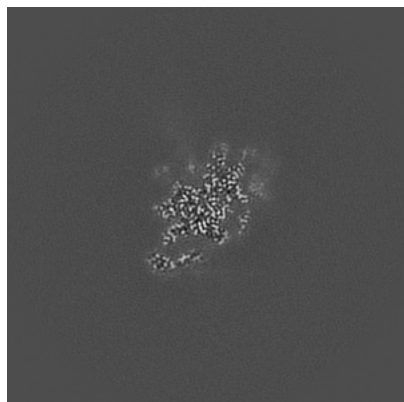


Z Index: 192

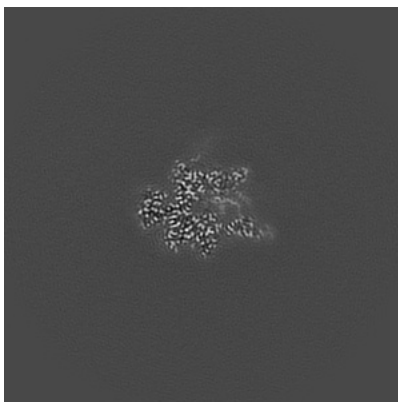
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

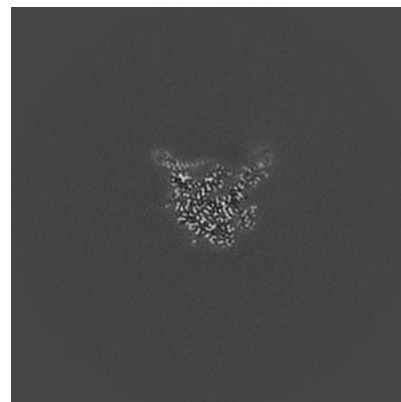
6.3.1 Primary map



X Index: 210

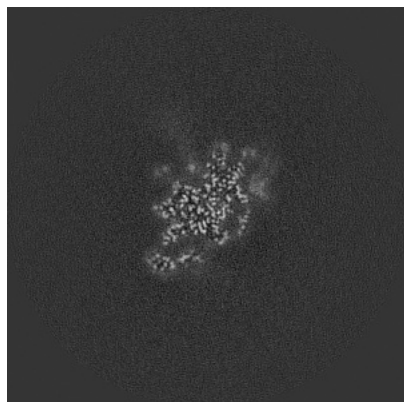


Y Index: 188

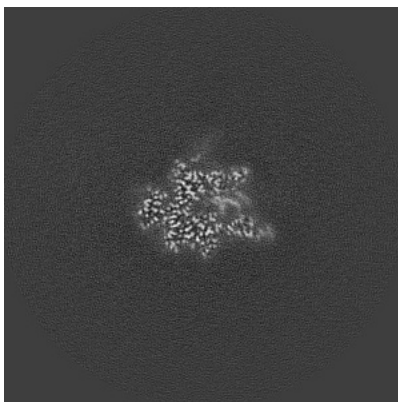


Z Index: 168

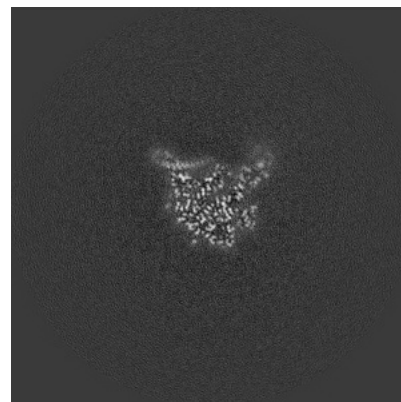
6.3.2 Raw map



X Index: 210



Y Index: 188

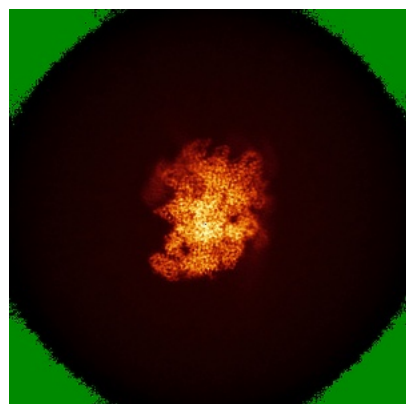


Z Index: 168

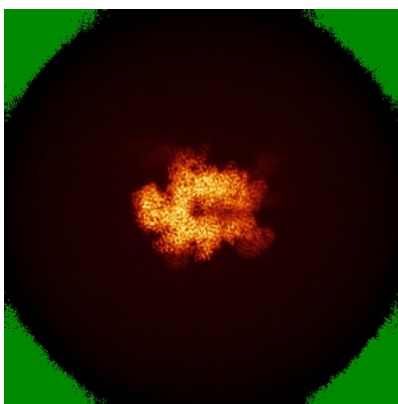
The images above show the largest variance slices of the map in three orthogonal directions.

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

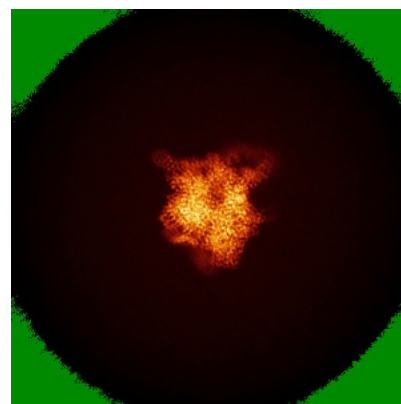
6.4.1 Primary map



X

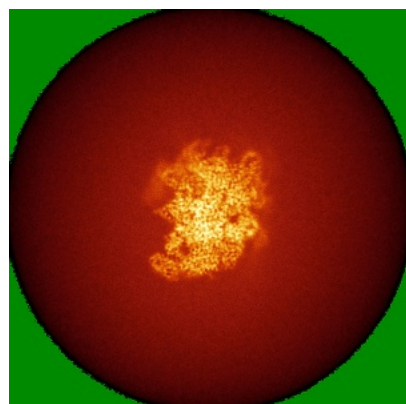


Y

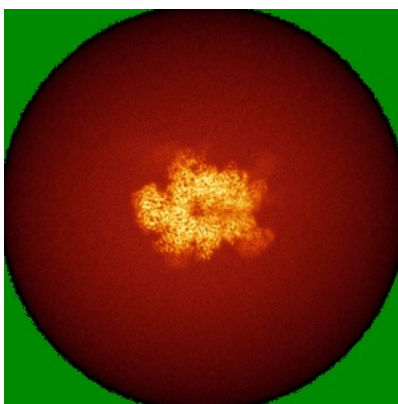


Z

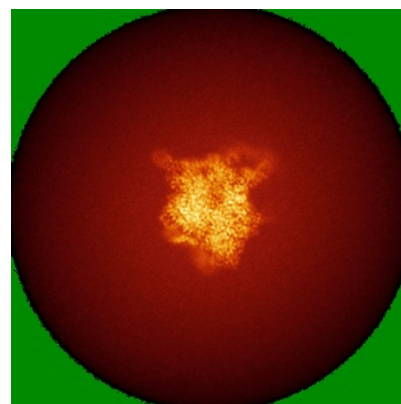
6.4.2 Raw map



X



Y

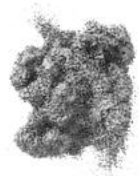


Z

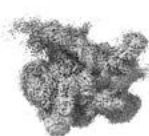
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.0033. 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.

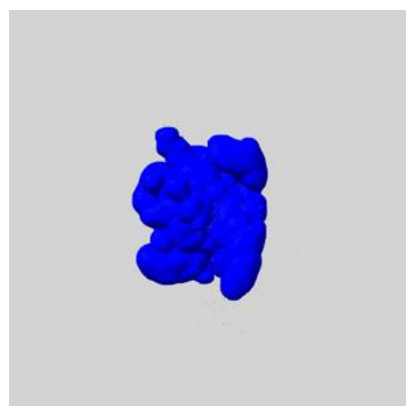
6.6 Mask visualisation [i](#)

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

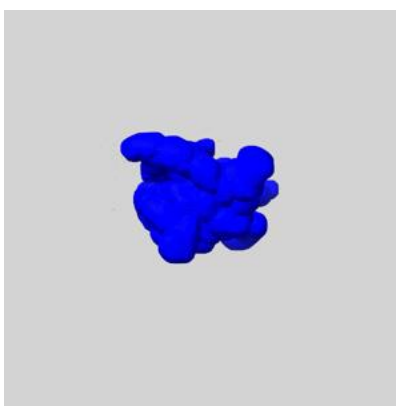
A mask typically either:

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

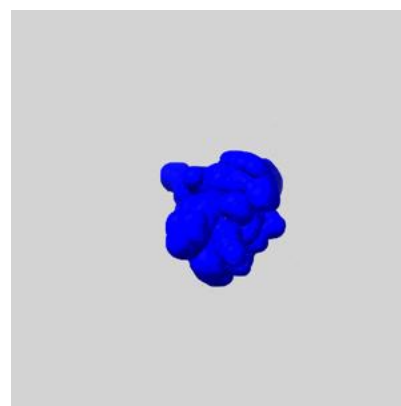
6.6.1 emd_71632_msk_1.map [i](#)



X



Y

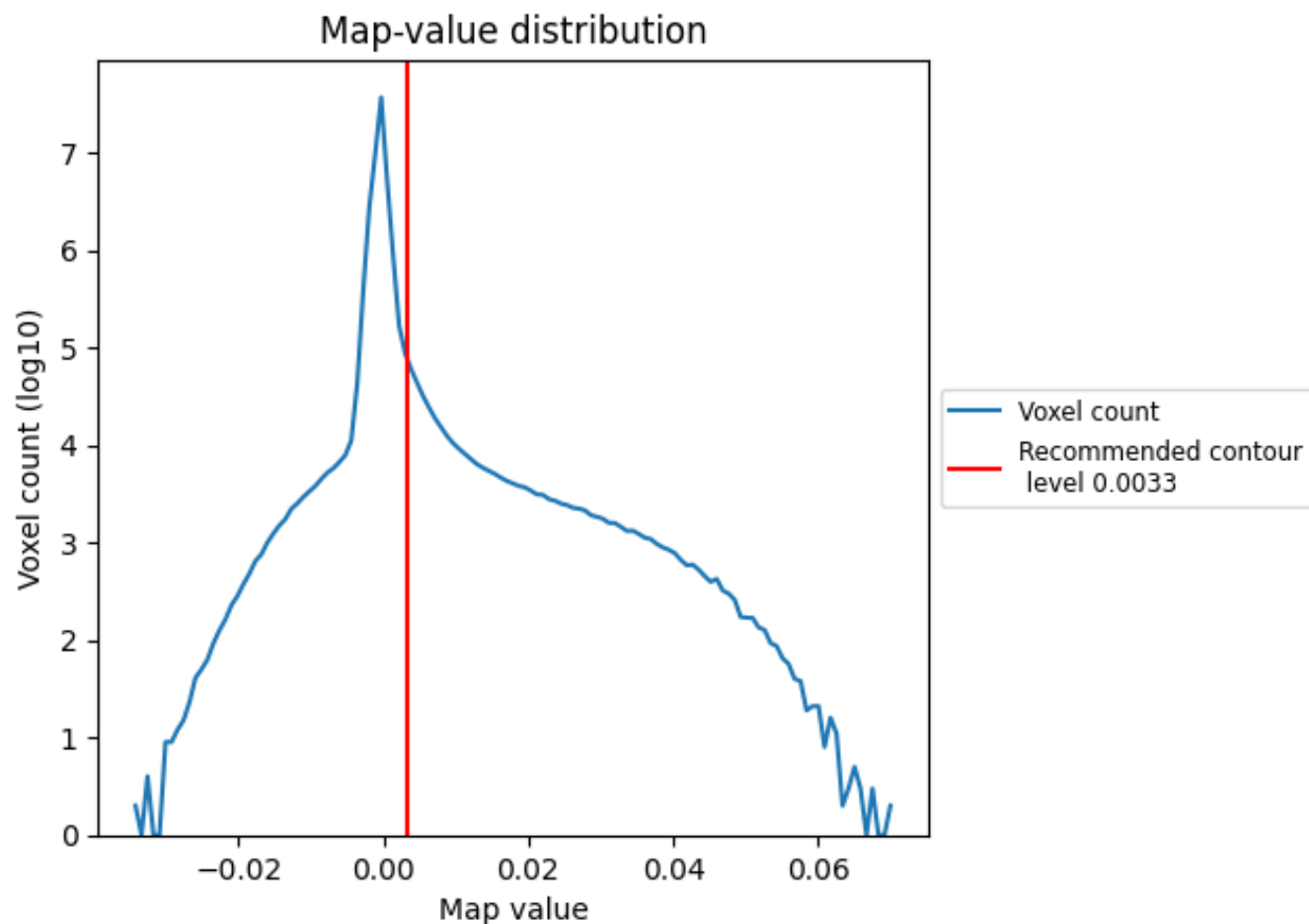


Z

7 Map analysis [i](#)

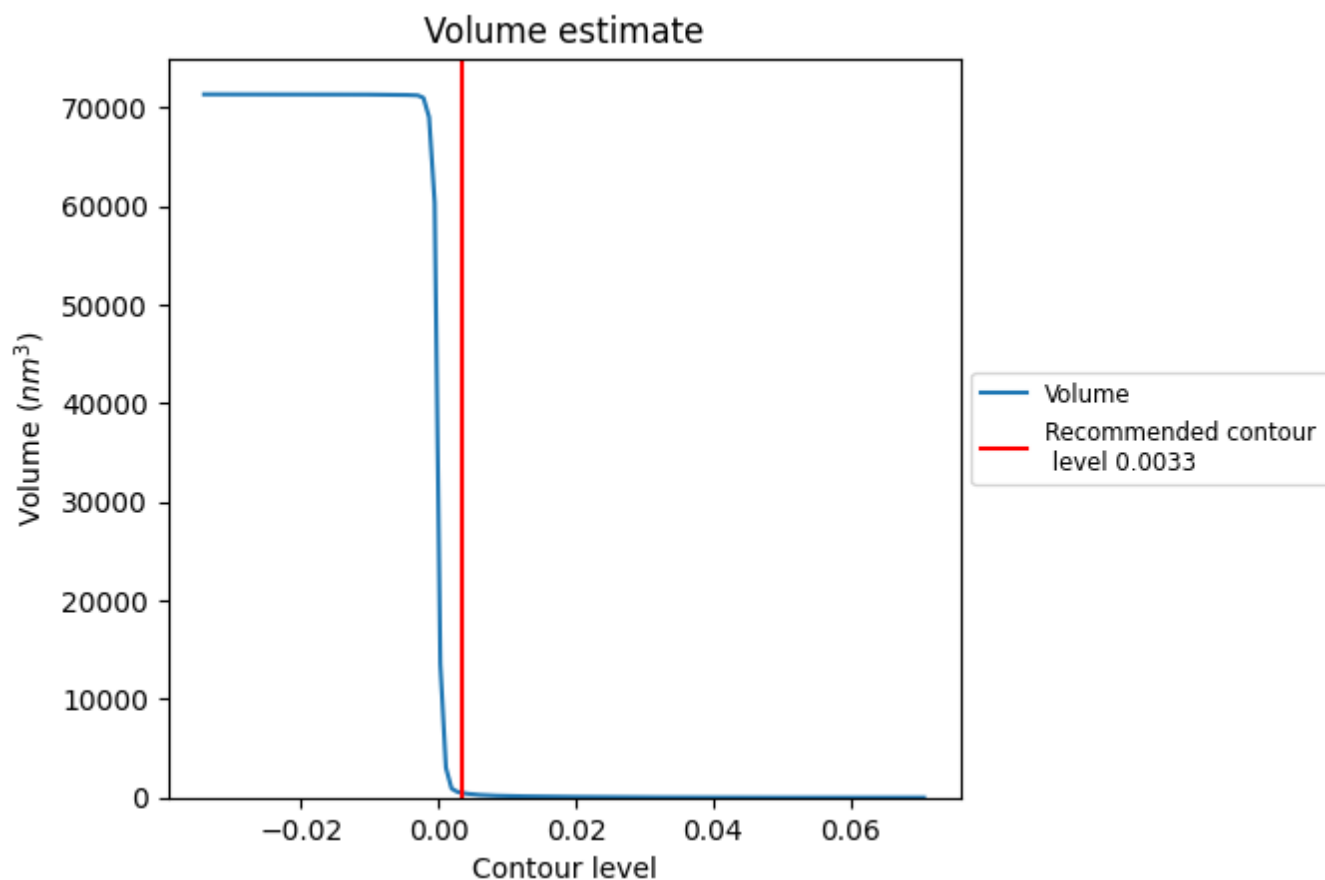
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

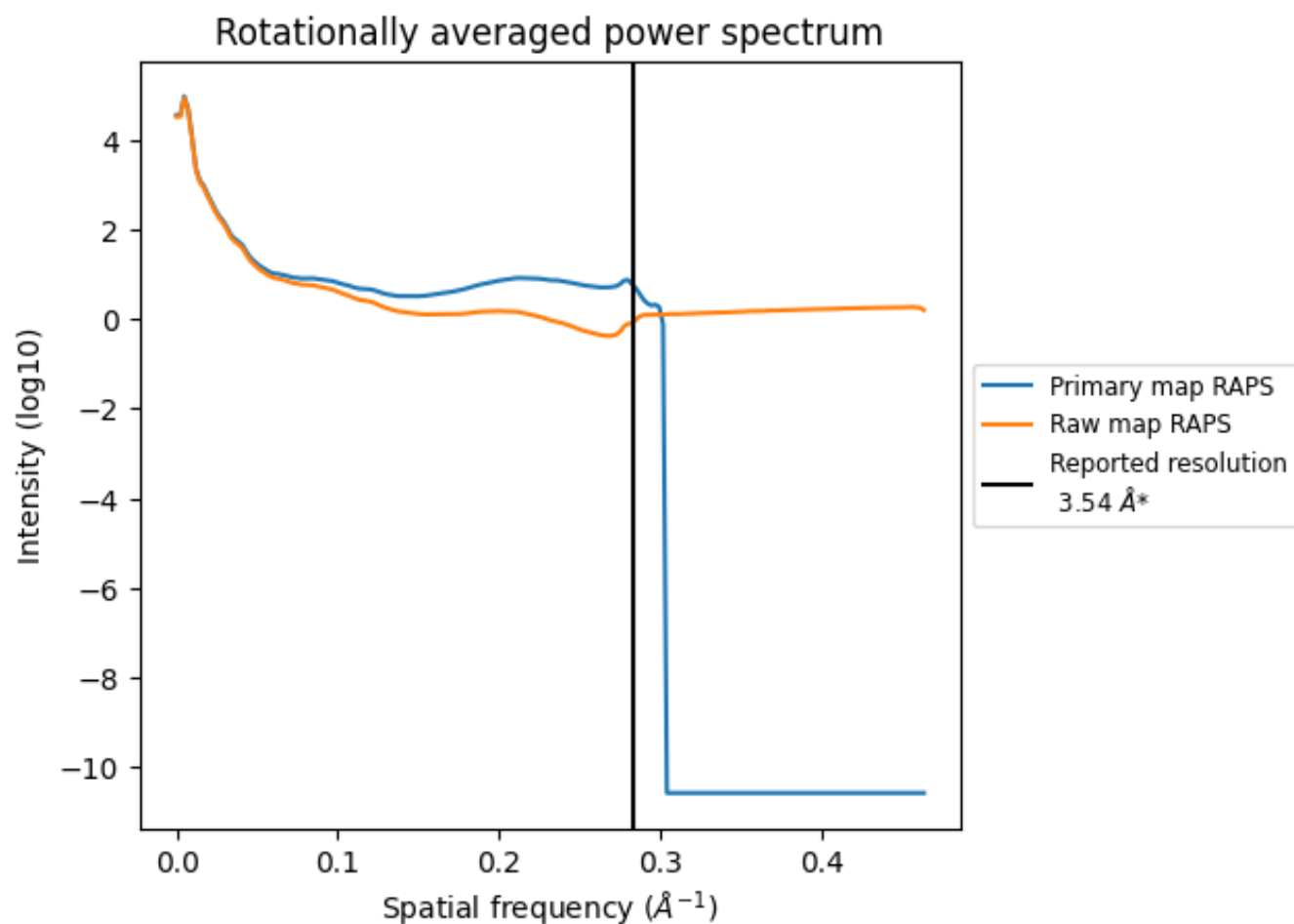
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 497 nm³; this corresponds to an approximate mass of 449 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 ⓘ

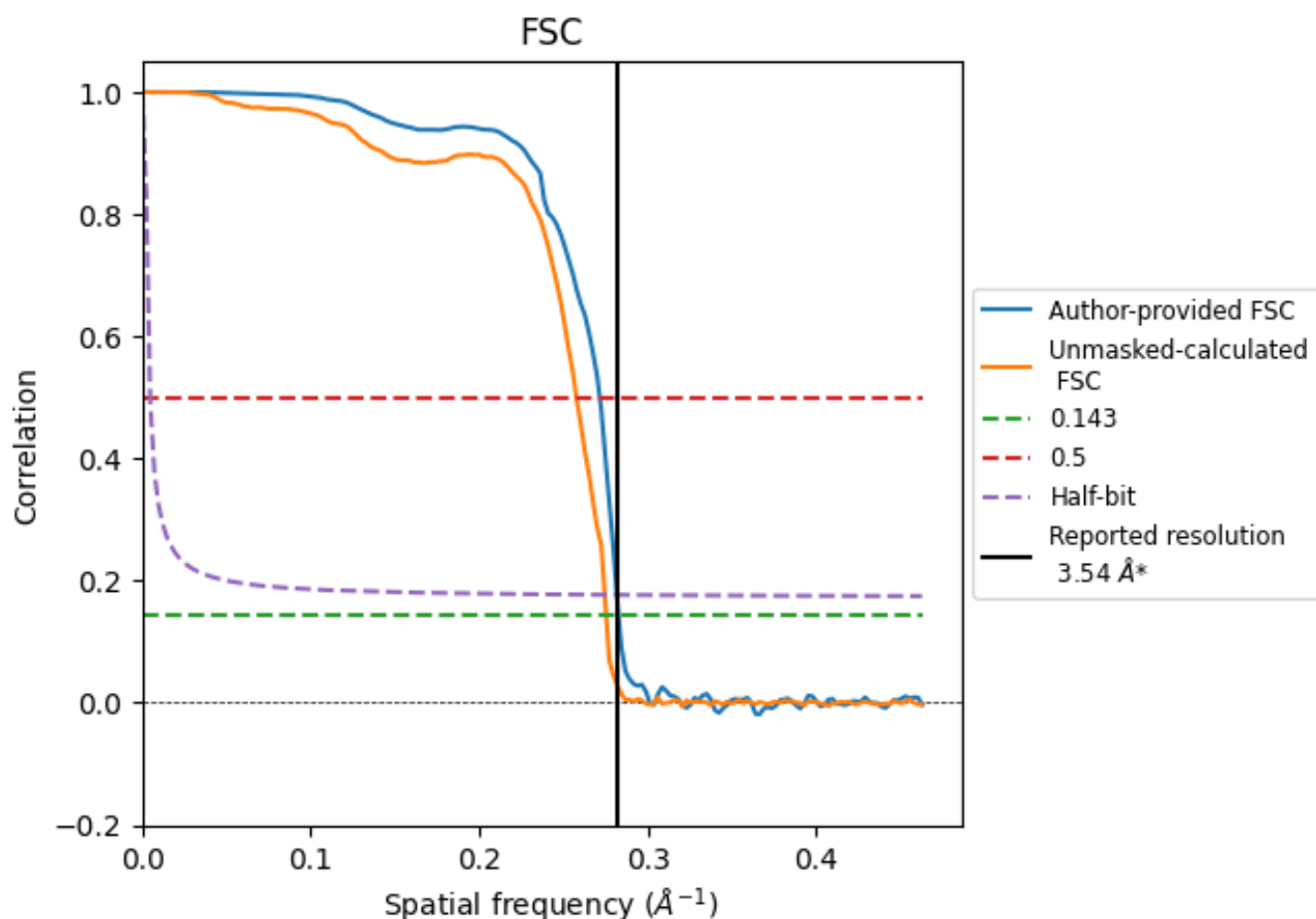


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 \AA^{-1}

8.2 Resolution estimates [i](#)

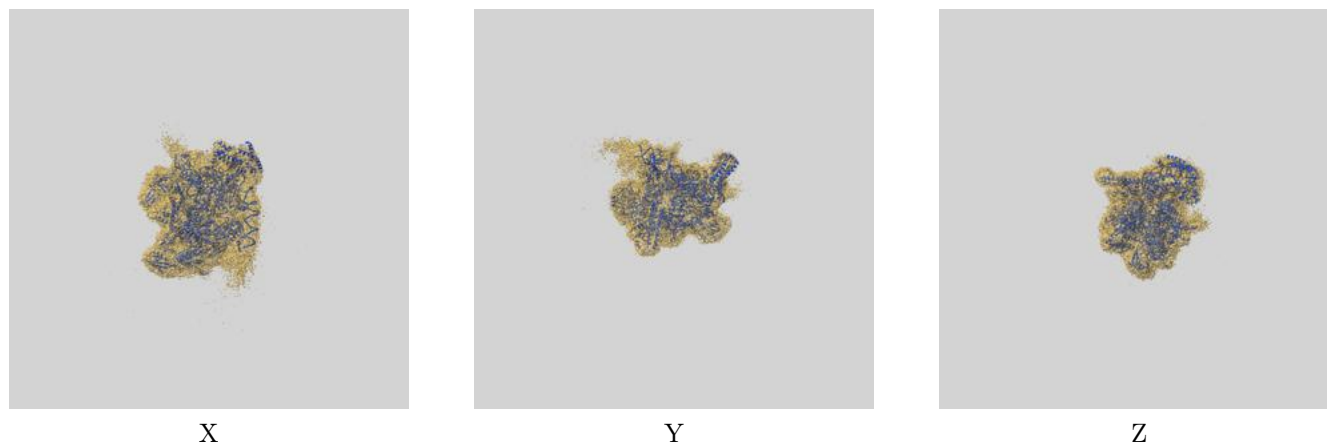
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.54	3.68	3.55
Unmasked-calculated*	3.63	3.88	3.64

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

9 Map-model fit [i](#)

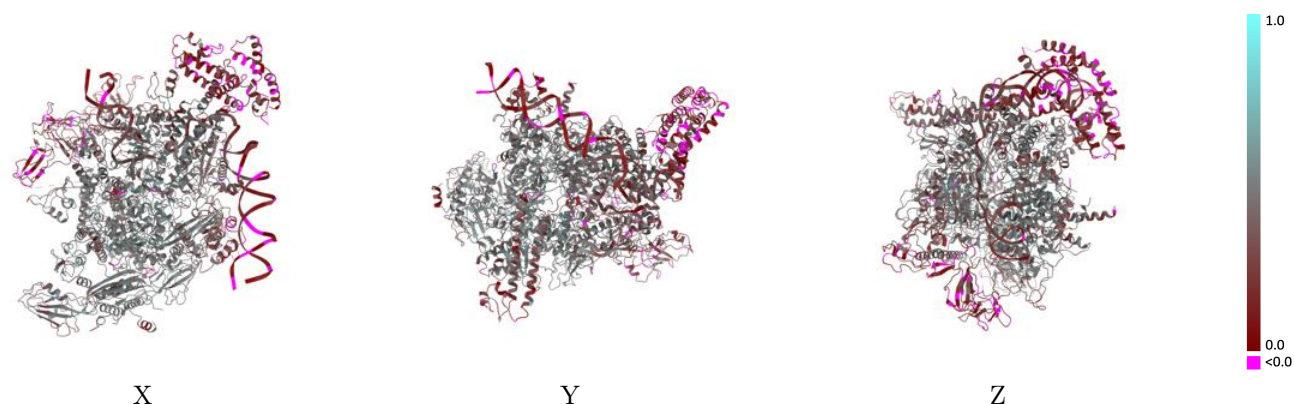
This section contains information regarding the fit between EMDB map EMD-71632 and PDB model 9PGH. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



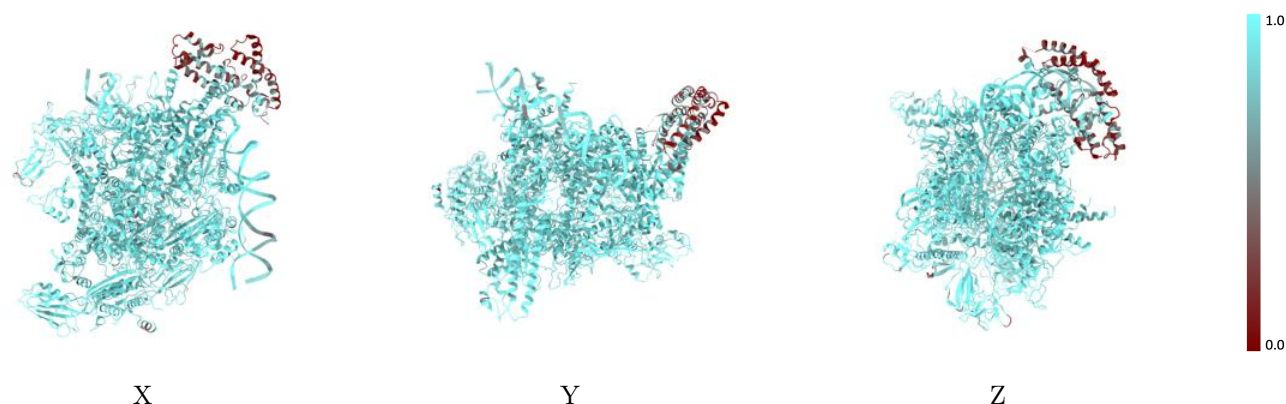
The images above show the 3D surface view of the map at the recommended contour level 0.0033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



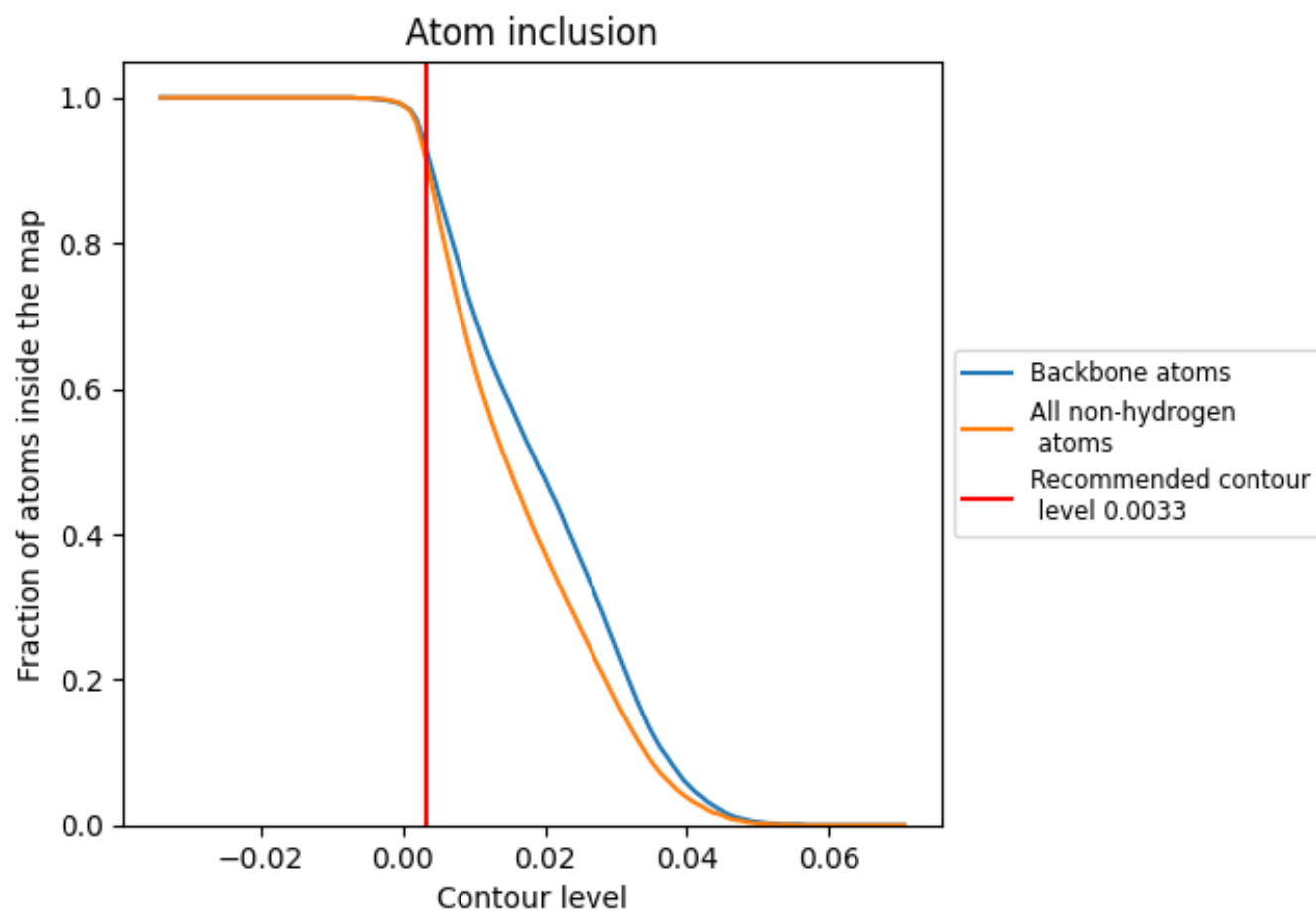
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0033).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (0.0033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9140</div>	<div><div></div>0.3860</div>
A	<div><div></div>0.9430</div>	<div><div></div>0.4510</div>
B	<div><div></div>0.9350</div>	<div><div></div>0.4290</div>
C	<div><div></div>0.9480</div>	<div><div></div>0.4240</div>
D	<div><div></div>0.9410</div>	<div><div></div>0.4160</div>
E	<div><div></div>0.9140</div>	<div><div></div>0.4140</div>
F	<div><div></div>0.7360</div>	<div><div></div>0.2570</div>
H	<div><div></div>0.9030</div>	<div><div></div>0.1940</div>
I	<div><div></div>0.8880</div>	<div><div></div>0.1500</div>

1.0

0.0

<0.0