



wwPDB EM Validation Summary Report ⓘ

May 29, 2025 – 04:54 pm BST

PDB ID : 9H2J / pdb_00009h2j
EMDB ID : EMD-51808
Title : AcMNPV apical cap - C14 anchor complex only
Authors : Effantin, G.; Kandiah, E.; Pelosse, M.
Deposited on : 2024-10-11
Resolution : 4.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

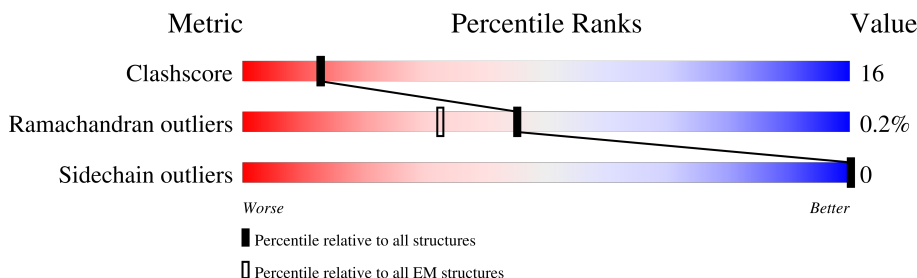
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	290	
1	B	290	
2	C	361	
2	D	361	
3	E	477	
4	F	347	
4	G	347	
4	L	347	

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Mol	Chain	Length	Quality of chain
4	M	347	
5	H	691	
5	I	691	
5	J	691	
6	K	390	
7	N	808	
7	P	808	
8	O	168	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28099 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 Occlusion-derived virus envelope protein E27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1977	1269	321	378	9		
1	B	184	Total	C	N	O	S	0	0
			1498	974	239	277	8		

- Molecule 2 is a protein called Protein C42.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	212	Total	C	N	O	S	0	0
			1752	1113	295	328	16		
2	D	191	Total	C	N	O	S	0	0
			1597	1018	271	293	15		

- Molecule 3 is a protein called Protein AC142.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	469	Total	C	N	O	S	0	0
			3855	2506	633	693	23		

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	214	Total	C	N	O	S	0	0
			1723	1093	297	321	12		
4	G	280	Total	C	N	O	S	0	0
			2254	1424	395	420	15		
4	L	124	Total	C	N	O	S	0	0
			997	642	171	179	5		
4	M	274	Total	C	N	O	S	0	0
			2219	1409	383	415	12		

- Molecule 5 is a protein called Capsid-associated protein VP80.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	214	Total	C	N	O	S	0	0
			1794	1162	300	318	14		
5	I	176	Total	C	N	O	S	0	0
			1462	947	242	261	12		
5	J	171	Total	C	N	O	S	0	0
			1430	932	238	248	12		

- Molecule 6 is a protein called Protein AC109.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	350	Total	C	N	O	S	0	0
			2856	1846	476	519	15		

- Molecule 7 is a protein called Protein Ac66.

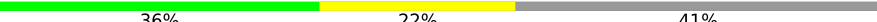
Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	77	Total	C	N	O	S	0	0
			655	401	120	133	1		
7	P	79	Total	C	N	O	S	0	0
			671	411	122	137	1		

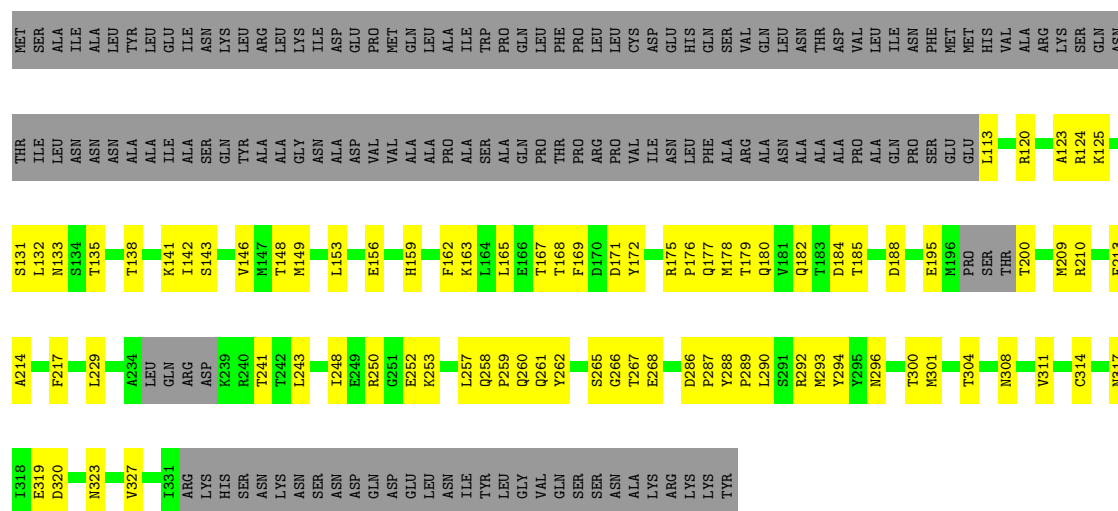
- Molecule 8 is a protein called Tyrosine-protein phosphatase.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	168	Total	C	N	O	S	0	0
			1356	871	232	244	9		


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

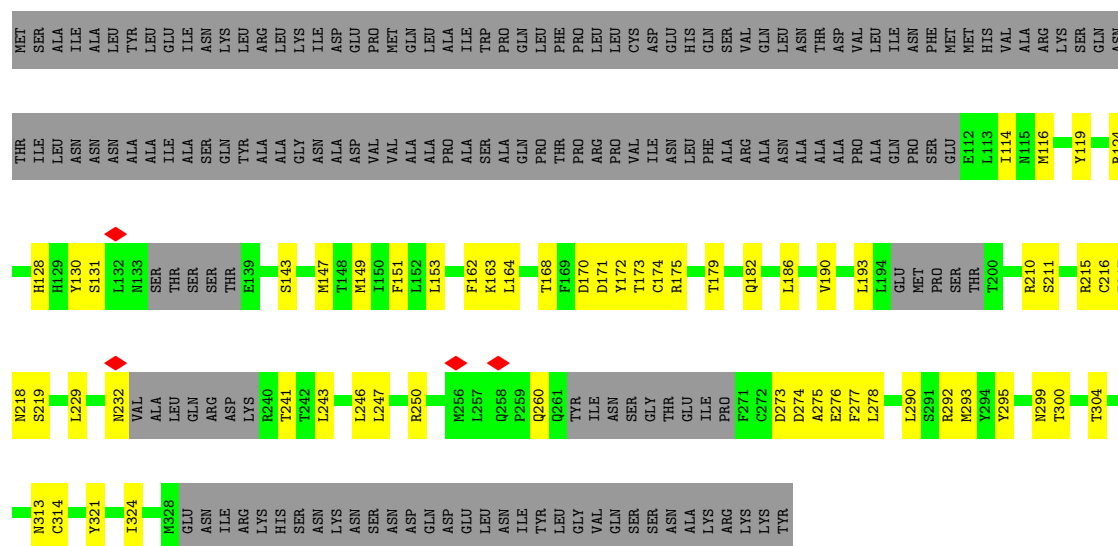
Mol	Chain	Residues	Atoms		AltConf
9	F	1	Total	Zn	0
			1	1	
9	G	1	Total	Zn	0
			1	1	
9	M	1	Total	Zn	0
			1	1	

Chain C:  36% 22% 41%



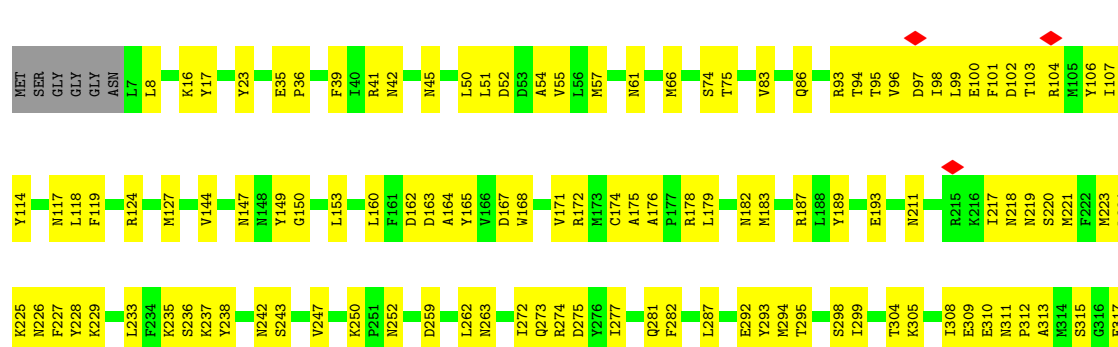
• Molecule 2: Protein C42

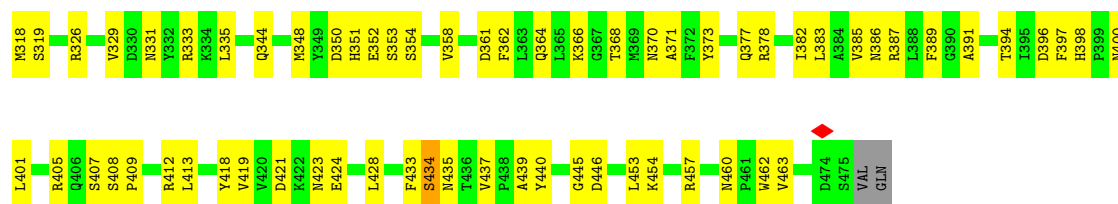
Chain D:  36% 17% 47%



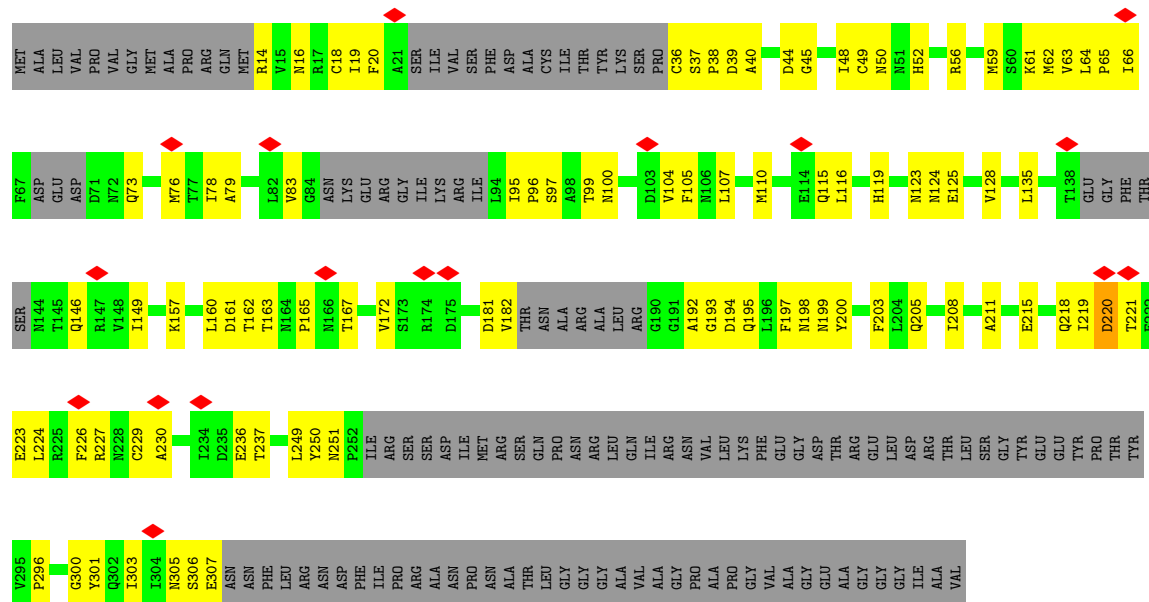
• Molecule 3: Protein AC142

Chain E:  61% 38% 1%

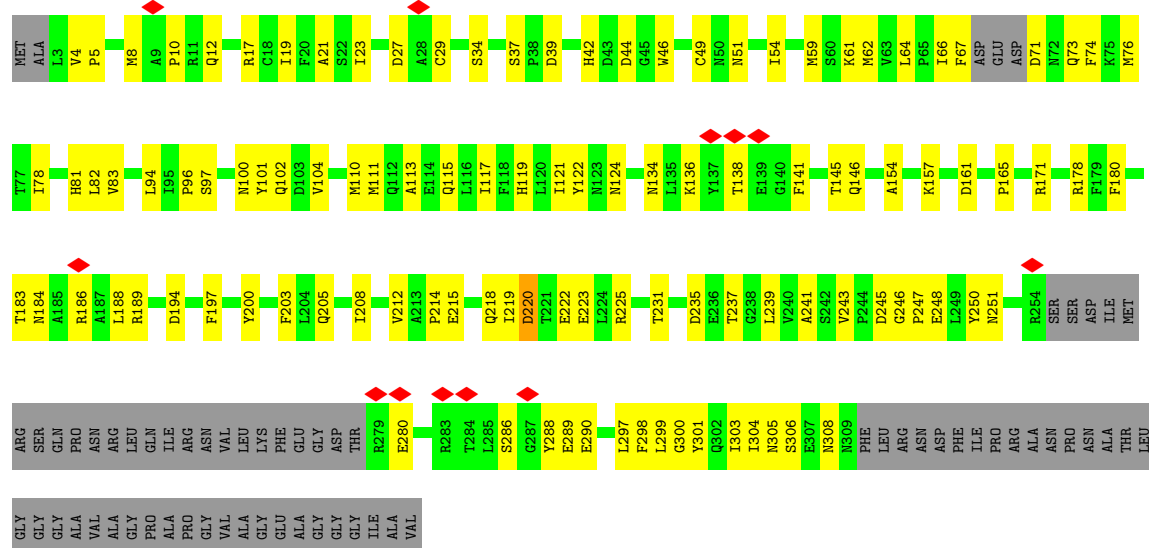




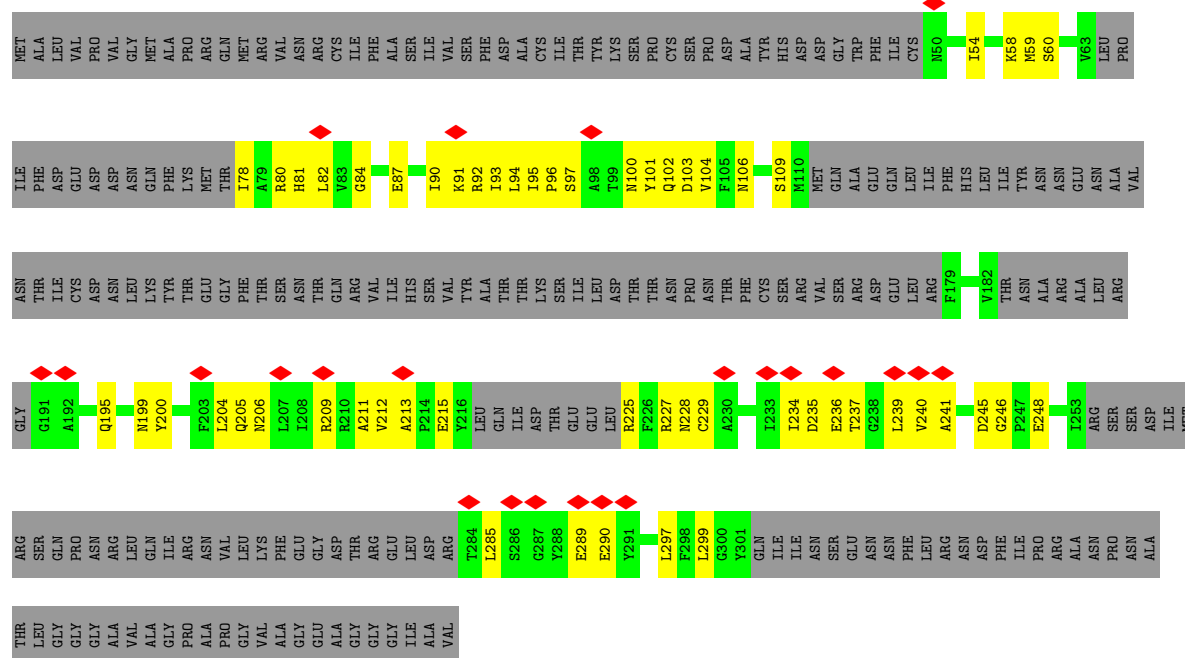
• Molecule 4: Major capsid protein



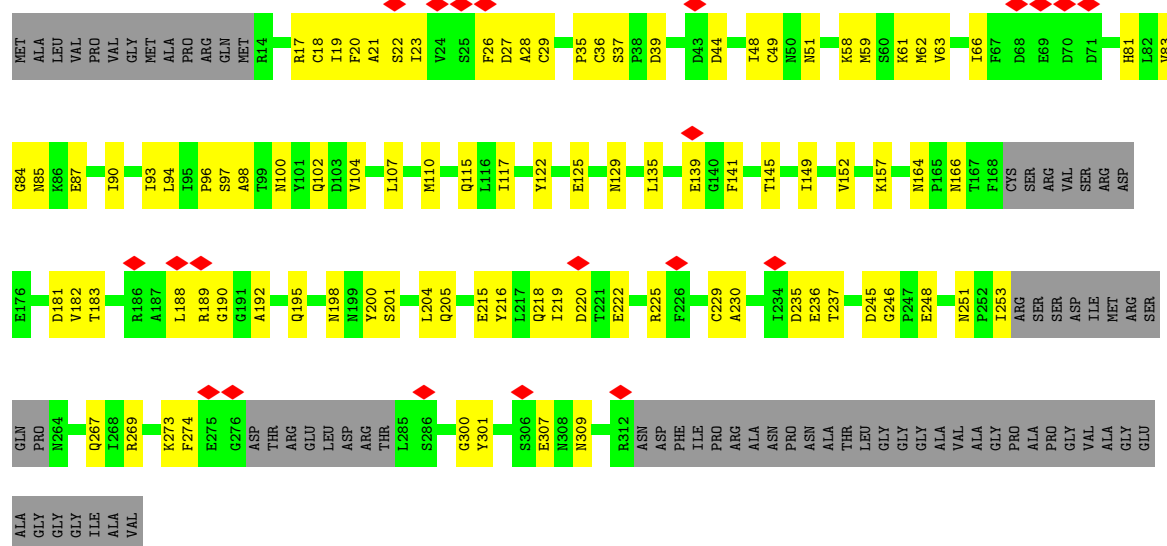
• Molecule 4: Major capsid protein



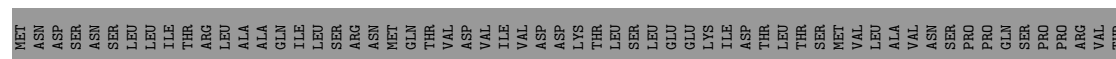
- Molecule 4: Major capsid protein

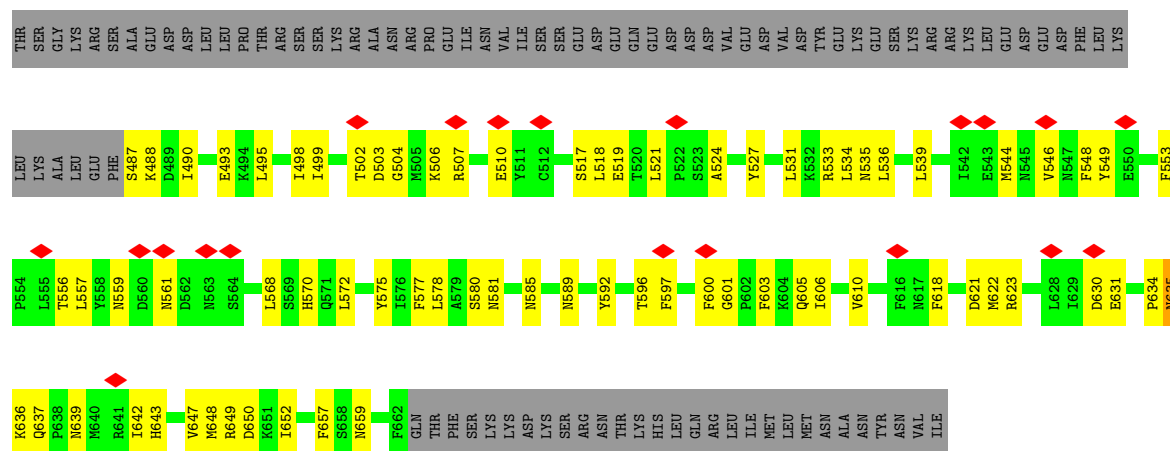


- Molecule 4: Major capsid protein



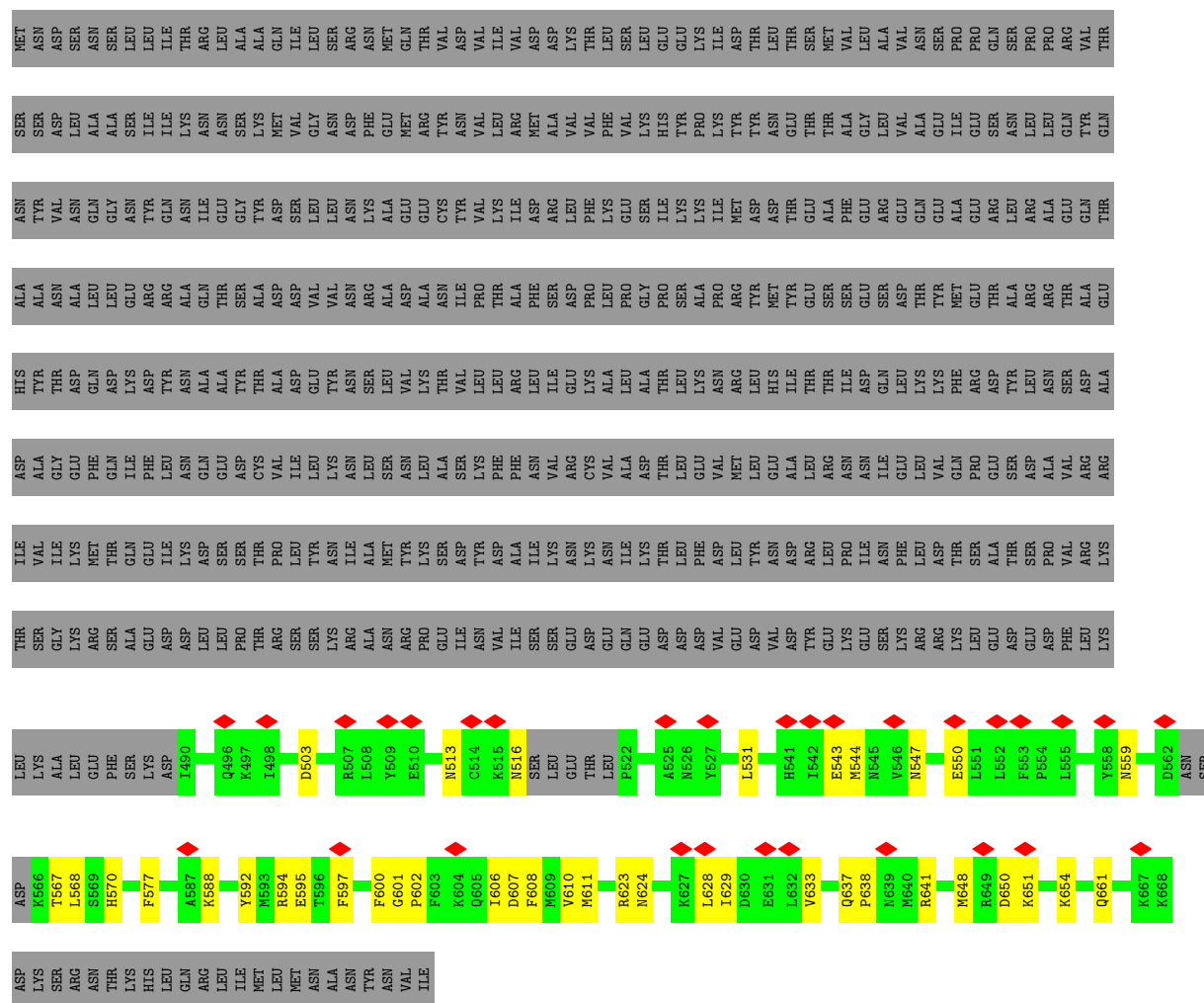
- Molecule 5: Capsid-associated protein VP80





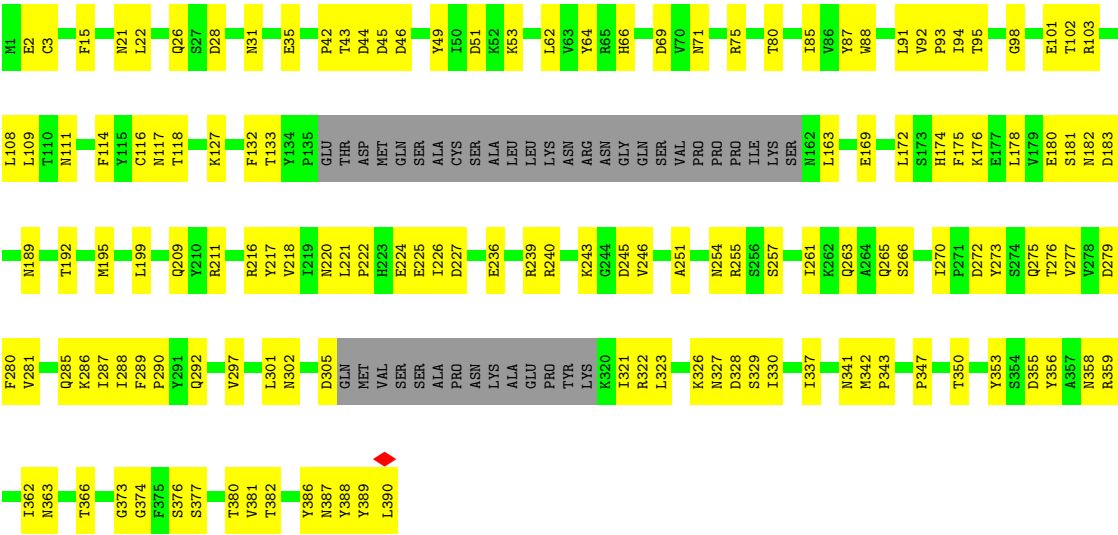
• Molecule 5: Capsid-associated protein VP80

Chain J: 19% 6% 75%

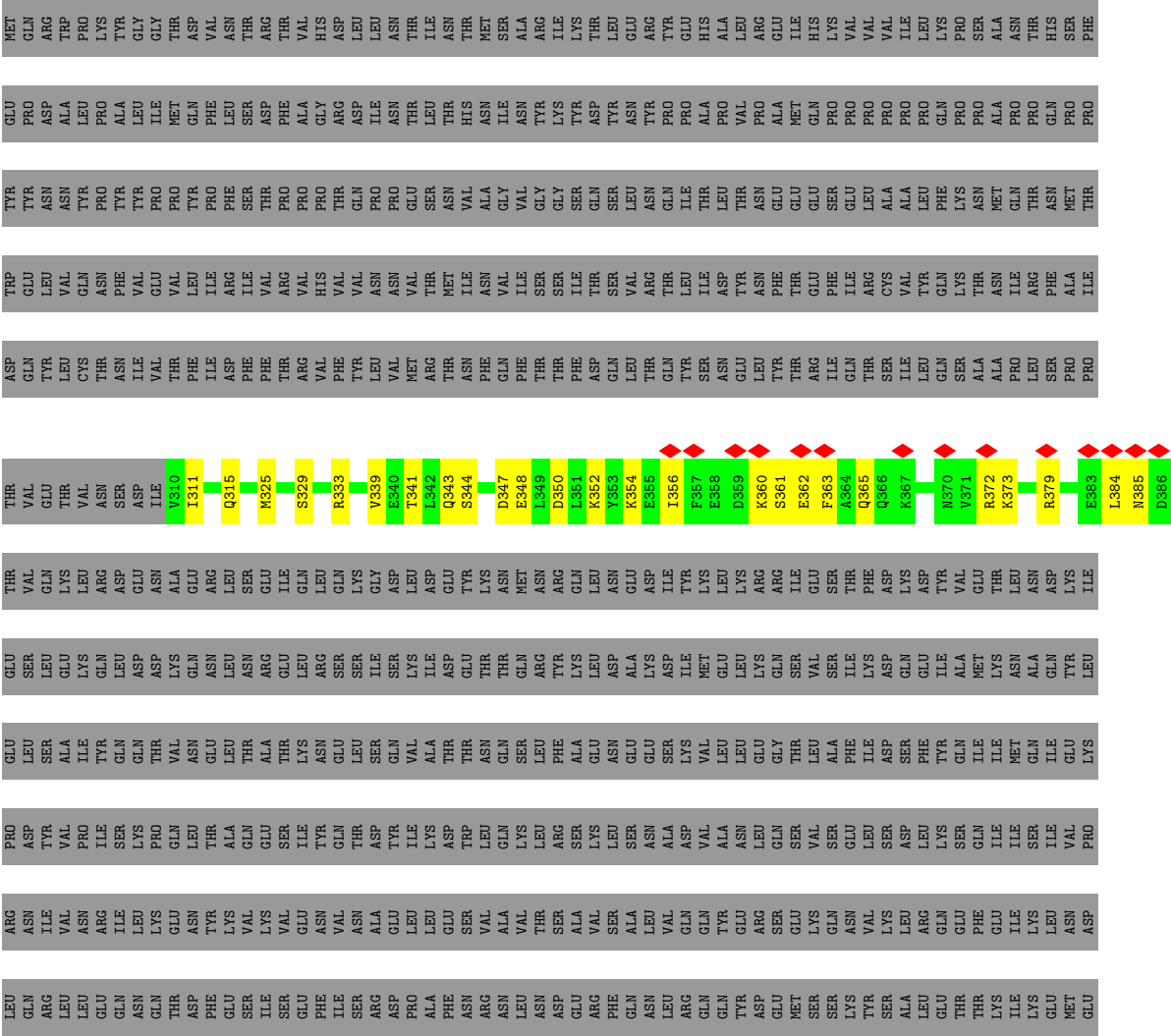


• Molecule 6: Protein AC109

Chain K: 54% 36% 10%



• Molecule 7: Protein Ac66



- Molecule 7: Protein Ac66



SER	GLU	MET	LYS	LEU	ASN	THR	GLN	LEU	ASP	GLU	LEU	ASN	SER	LEU	PHE	VAL	LYS	TYR	ASN	ARG	ALA	GLN	ILE	PHE	GLU	TRP	LYS	THR	SER	MET	LYS	ARG	TYR	GLU	THR	LEU	ALA	ARG	THR	THR	ALA	ALA	SER	VAL	GLN	PRO	ASN	VAL	GLU
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- Molecule 8: Tyrosine-protein phosphatase



M1	F2	P3	A4	H7	Q11	G12	G13	Q14	V15	I16	K17	D18	S19	N20	L21	L22	T26	P27	L28	E31	L32	F33	T37	E40	D41	V42	N52	I55	G56	A57	I58	X66	Y67	Y68	D69	G70	V71	L78	I83	G87	X88	T89	L90	E93	S94	T95
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C14	Depositor
Number of particles used	8327	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0065	Depositor
Map size (Å)	675.0, 675.0, 675.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2010	0.36	0/2713
1	B	0.14	0/1523	0.32	0/2052
2	C	0.24	0/1782	0.34	0/2404
2	D	0.19	0/1623	0.32	0/2184
3	E	0.26	0/3954	0.39	0/5354
4	F	0.15	0/1755	0.30	0/2374
4	G	0.21	0/2300	0.36	0/3116
4	L	0.12	0/1016	0.27	0/1368
4	M	0.19	0/2264	0.33	0/3065
5	H	0.22	0/1828	0.33	0/2456
5	I	0.17	0/1493	0.35	0/2013
5	J	0.15	0/1460	0.31	0/1962
6	K	0.26	0/2928	0.34	0/3980
7	N	0.17	0/659	0.32	0/877
7	P	0.21	0/675	0.39	0/899
8	O	0.16	0/1389	0.32	0/1883
All	All	0.21	0/28659	0.34	0/38700

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1977	0	2001	97	0
1	B	1498	0	1517	39	0
2	C	1752	0	1752	72	0
2	D	1597	0	1597	51	0
3	E	3855	0	3851	158	0
4	F	1723	0	1670	73	0
4	G	2254	0	2209	76	0
4	L	997	0	983	50	0
4	M	2219	0	2163	67	0
5	H	1794	0	1810	55	0
5	I	1462	0	1464	55	0
5	J	1430	0	1441	29	0
6	K	2856	0	2852	128	0
7	N	655	0	653	22	0
7	P	671	0	668	21	0
8	O	1356	0	1358	40	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	M	1	0	0	0	0
All	All	28099	0	27989	914	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 16.

The worst 5 of 914 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:A:89:ALA:HA	1:A:102:PHE:CE2	1.43	1.52
1:A:89:ALA:CA	1:A:102:PHE:HE2	1.44	1.31
1:A:92:HIS:CB	1:A:102:PHE:CZ	2.22	1.21
1:A:92:HIS:HB2	1:A:102:PHE:CZ	1.78	1.18
3:E:102:ASP:OD2	3:E:172:ARG:HB3	1.45	1.13

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/290 (82%)	213 (90%)	25 (10%)	0	100	100
1	B	172/290 (59%)	164 (95%)	8 (5%)	0	100	100
2	C	206/361 (57%)	190 (92%)	16 (8%)	0	100	100
2	D	181/361 (50%)	169 (93%)	11 (6%)	1 (1%)	22	60
3	E	467/477 (98%)	404 (86%)	62 (13%)	1 (0%)	44	78
4	F	200/347 (58%)	177 (88%)	22 (11%)	1 (0%)	25	64
4	G	274/347 (79%)	242 (88%)	31 (11%)	1 (0%)	30	68
4	L	112/347 (32%)	108 (96%)	4 (4%)	0	100	100
4	M	266/347 (77%)	234 (88%)	32 (12%)	0	100	100
5	H	208/691 (30%)	195 (94%)	13 (6%)	0	100	100
5	I	174/691 (25%)	156 (90%)	17 (10%)	1 (1%)	22	60
5	J	165/691 (24%)	153 (93%)	12 (7%)	0	100	100
6	K	344/390 (88%)	319 (93%)	25 (7%)	0	100	100
7	N	75/808 (9%)	75 (100%)	0	0	100	100
7	P	77/808 (10%)	77 (100%)	0	0	100	100
8	O	166/168 (99%)	158 (95%)	8 (5%)	0	100	100
All	All	3325/7414 (45%)	3034 (91%)	286 (9%)	5 (0%)	45	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	434	SER
2	D	276	GLU
4	F	220	ASP
5	I	635	ASN
4	G	220	ASP

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	228/273 (84%)	228 (100%)	0	100	100
1	B	170/273 (62%)	170 (100%)	0	100	100
2	C	200/326 (61%)	200 (100%)	0	100	100
2	D	181/326 (56%)	181 (100%)	0	100	100
3	E	435/440 (99%)	435 (100%)	0	100	100
4	F	193/299 (64%)	193 (100%)	0	100	100
4	G	251/299 (84%)	251 (100%)	0	100	100
4	L	108/299 (36%)	108 (100%)	0	100	100
4	M	246/299 (82%)	246 (100%)	0	100	100
5	H	203/634 (32%)	203 (100%)	0	100	100
5	I	167/634 (26%)	167 (100%)	0	100	100
5	J	162/634 (26%)	162 (100%)	0	100	100
6	K	331/366 (90%)	331 (100%)	0	100	100
7	N	74/758 (10%)	74 (100%)	0	100	100
7	P	76/758 (10%)	76 (100%)	0	100	100
8	O	149/149 (100%)	149 (100%)	0	100	100
All	All	3174/6767 (47%)	3174 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
5	I	661	GLN
6	K	122	HIS
7	N	313	ASN
5	J	617	ASN
6	K	234	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

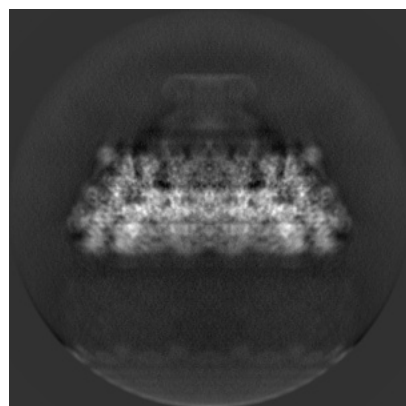
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51808. These allow visual inspection of the internal detail of the map and identification of artifacts.

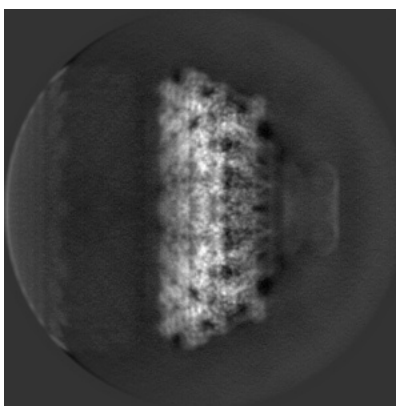
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

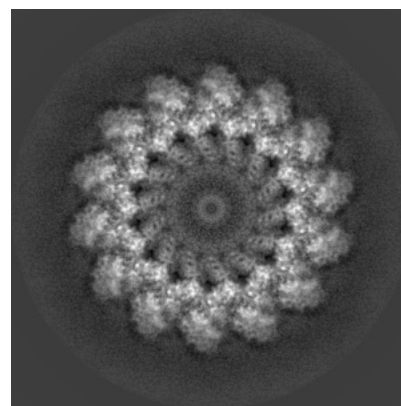
6.1.1 Primary map



X

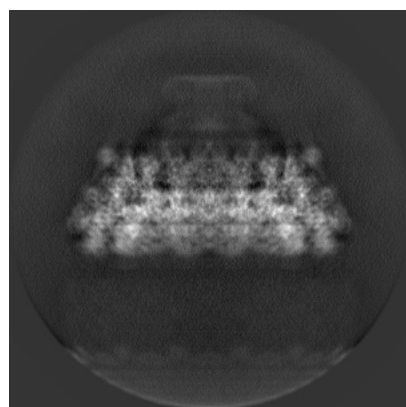


Y

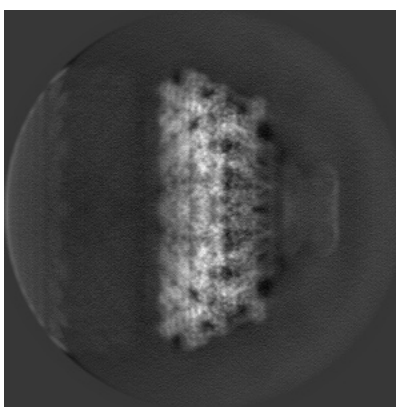


Z

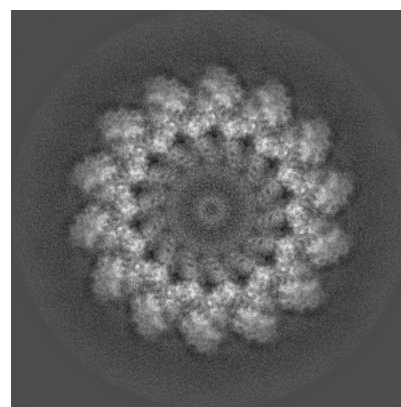
6.1.2 Raw map



X



Y

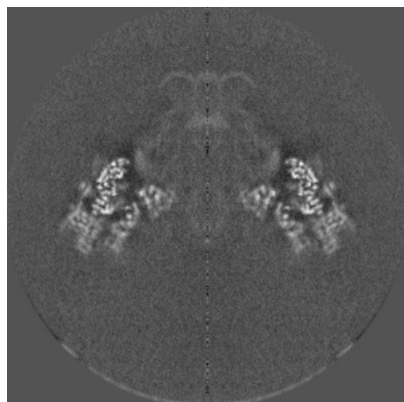


Z

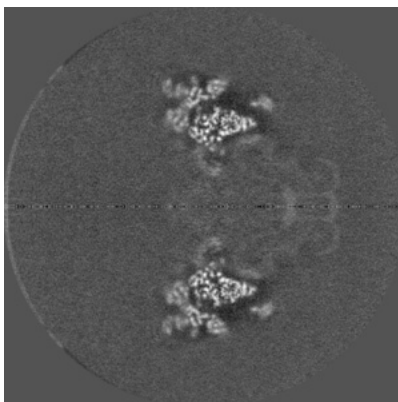
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

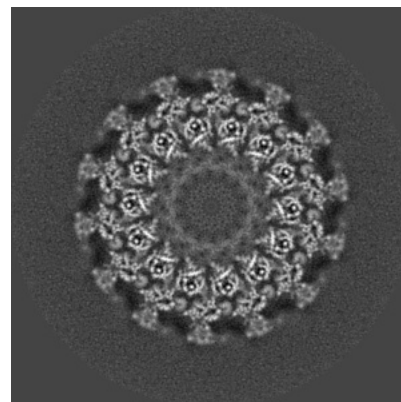
6.2.1 Primary map



X Index: 250

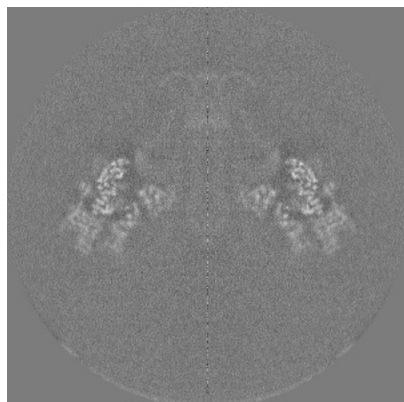


Y Index: 250

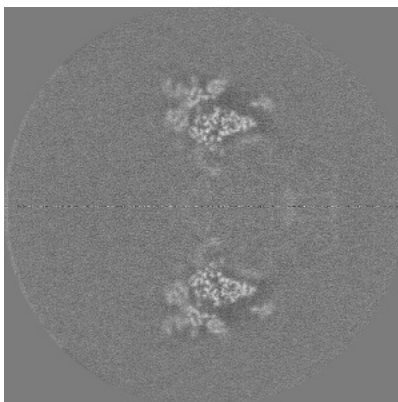


Z Index: 250

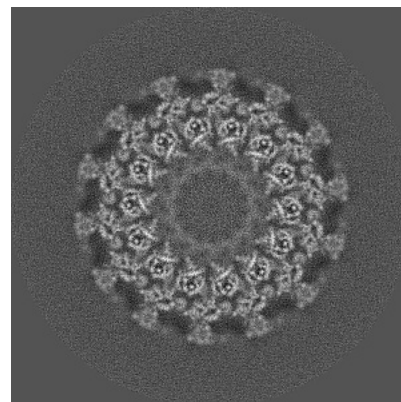
6.2.2 Raw map



X Index: 250



Y Index: 250

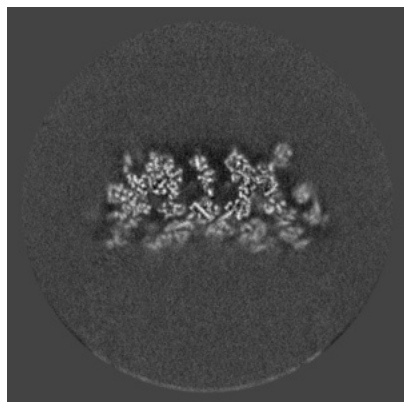


Z Index: 250

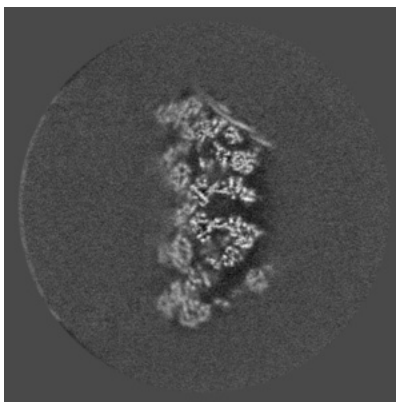
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

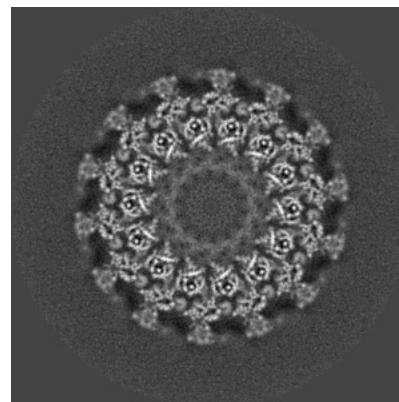
6.3.1 Primary map



X Index: 346

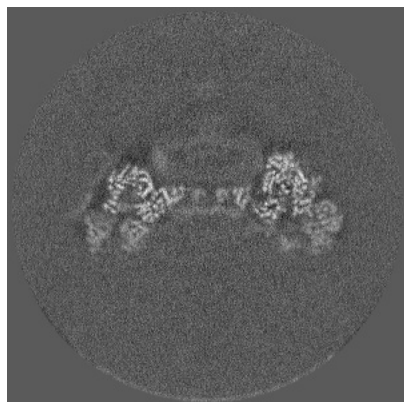


Y Index: 154

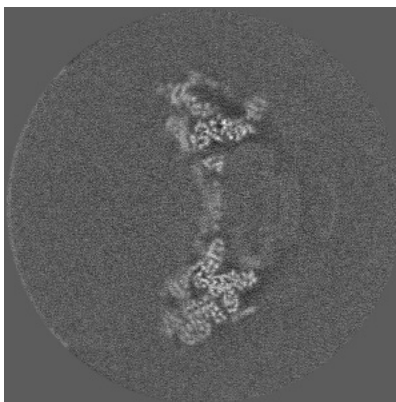


Z Index: 250

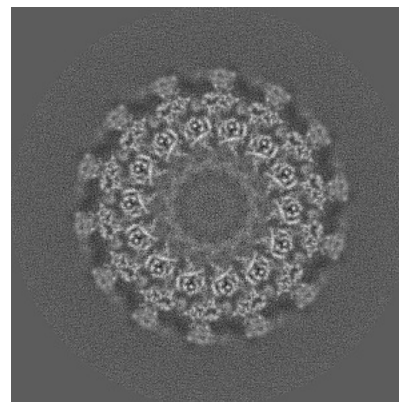
6.3.2 Raw map



X Index: 192



Y Index: 296

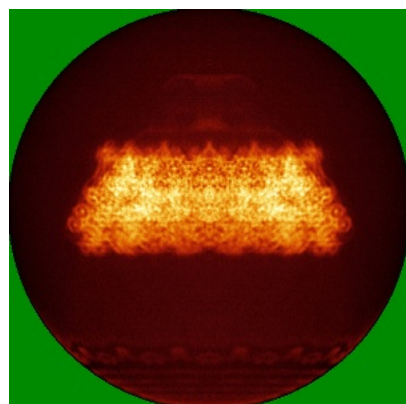


Z Index: 249

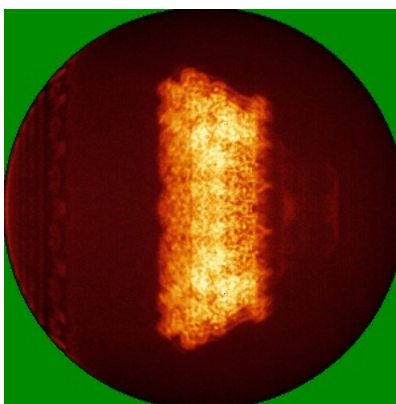
The images above show the largest variance slices of the map in three orthogonal directions.

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

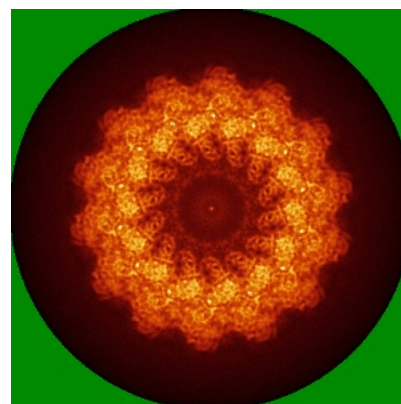
6.4.1 Primary map



X

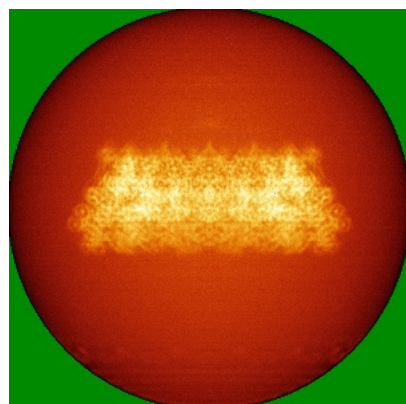


Y

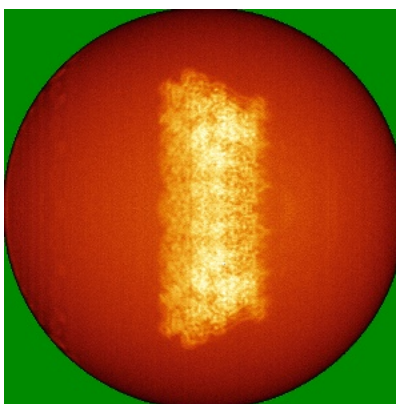


Z

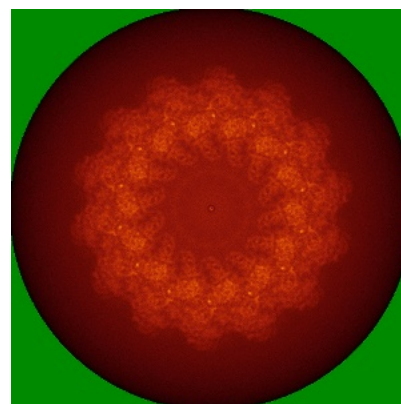
6.4.2 Raw map



X



Y

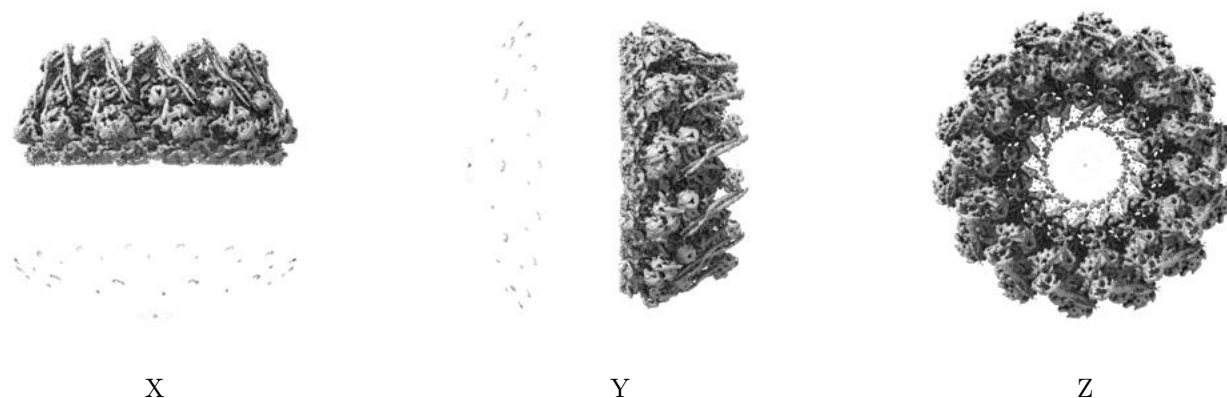


Z

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.

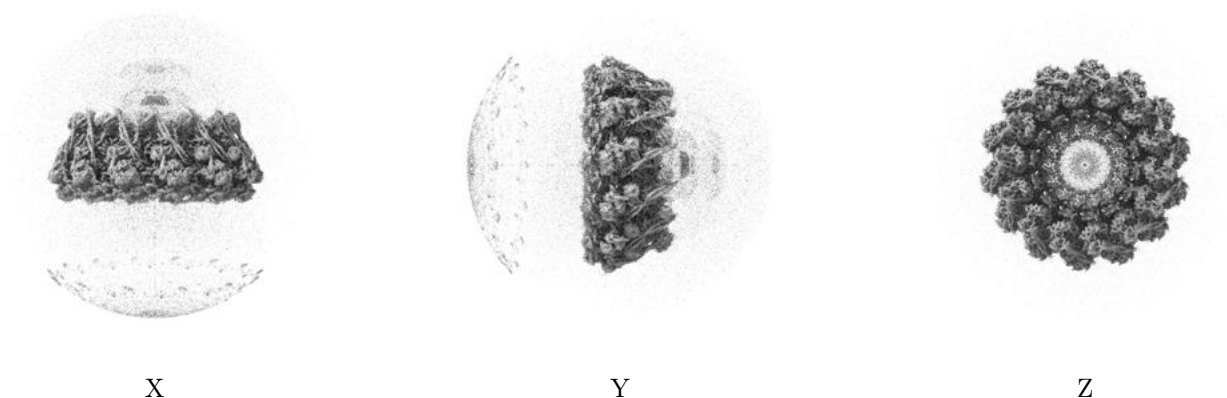
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0065. 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.

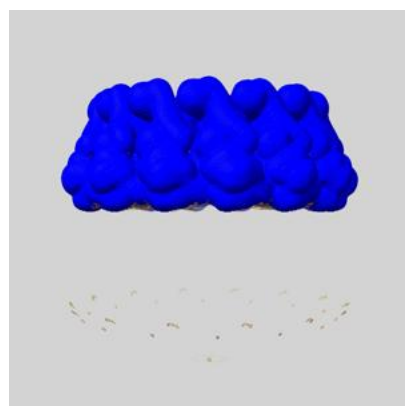
6.6 Mask visualisation [i](#)

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

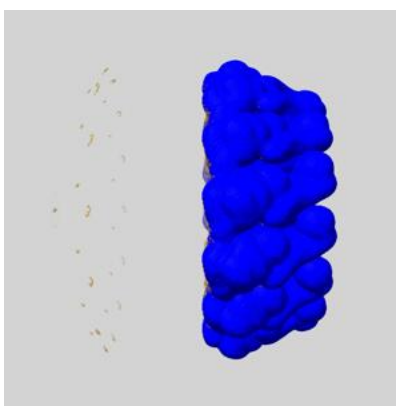
A mask typically either:

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

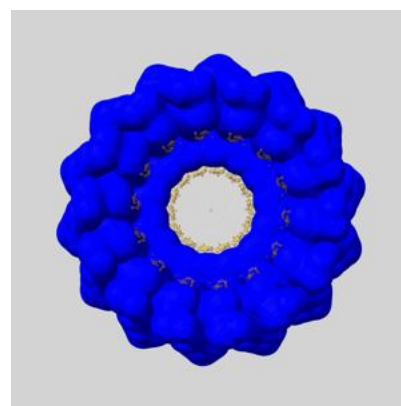
6.6.1 emd_51808_msk_1.map [i](#)



X



Y

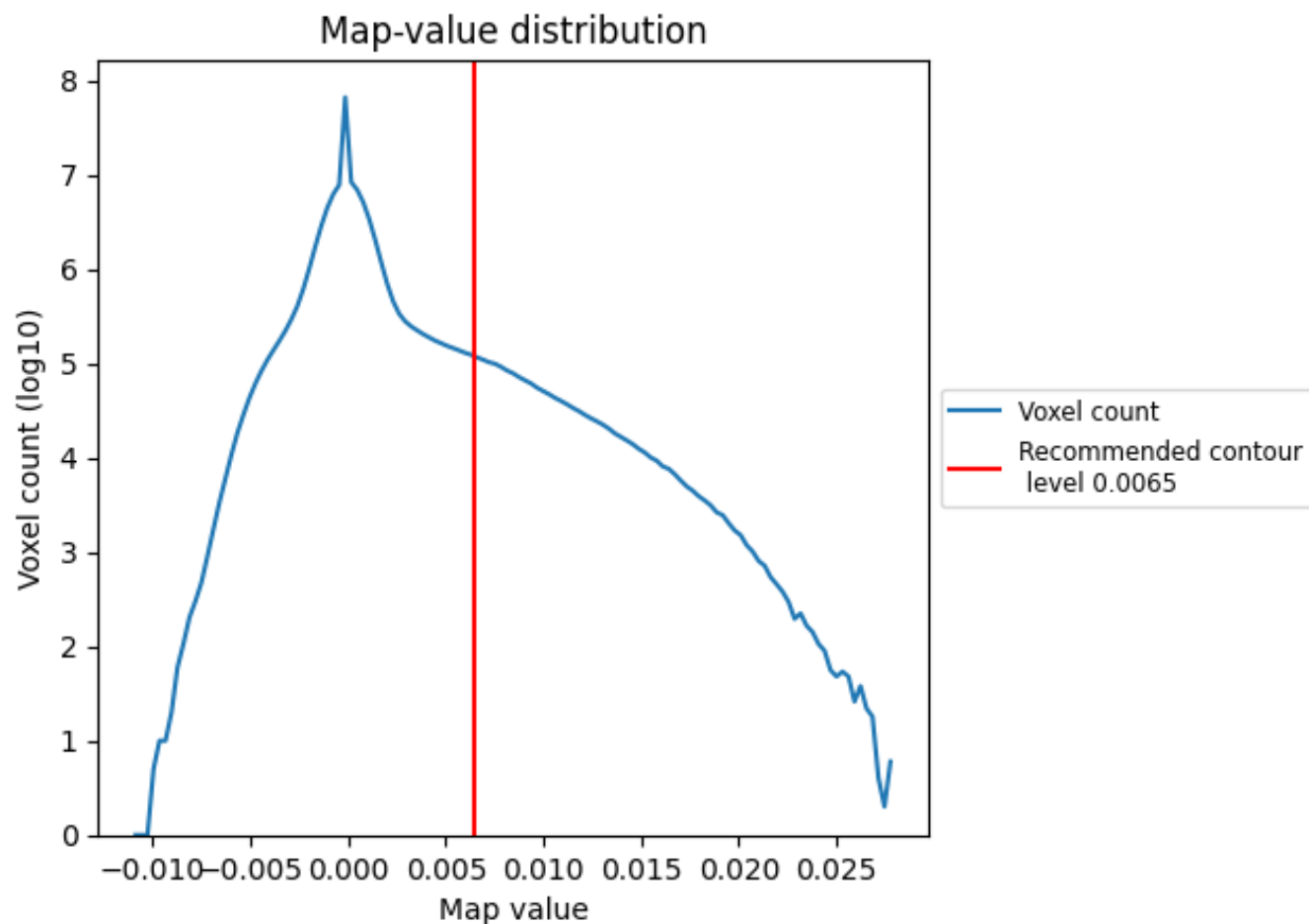


Z

7 Map analysis [i](#)

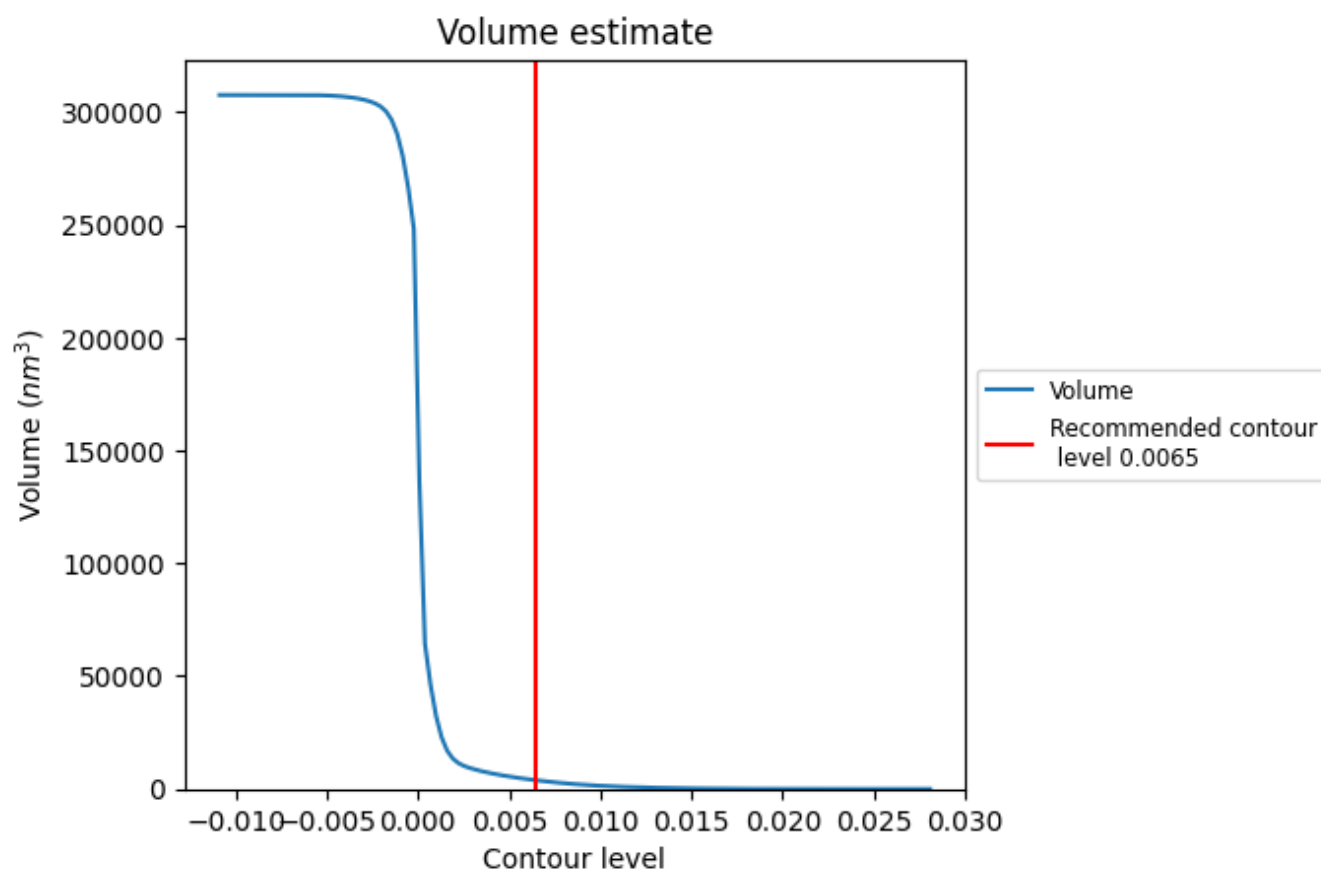
This section contains the results of statistical analysis of the map.

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.

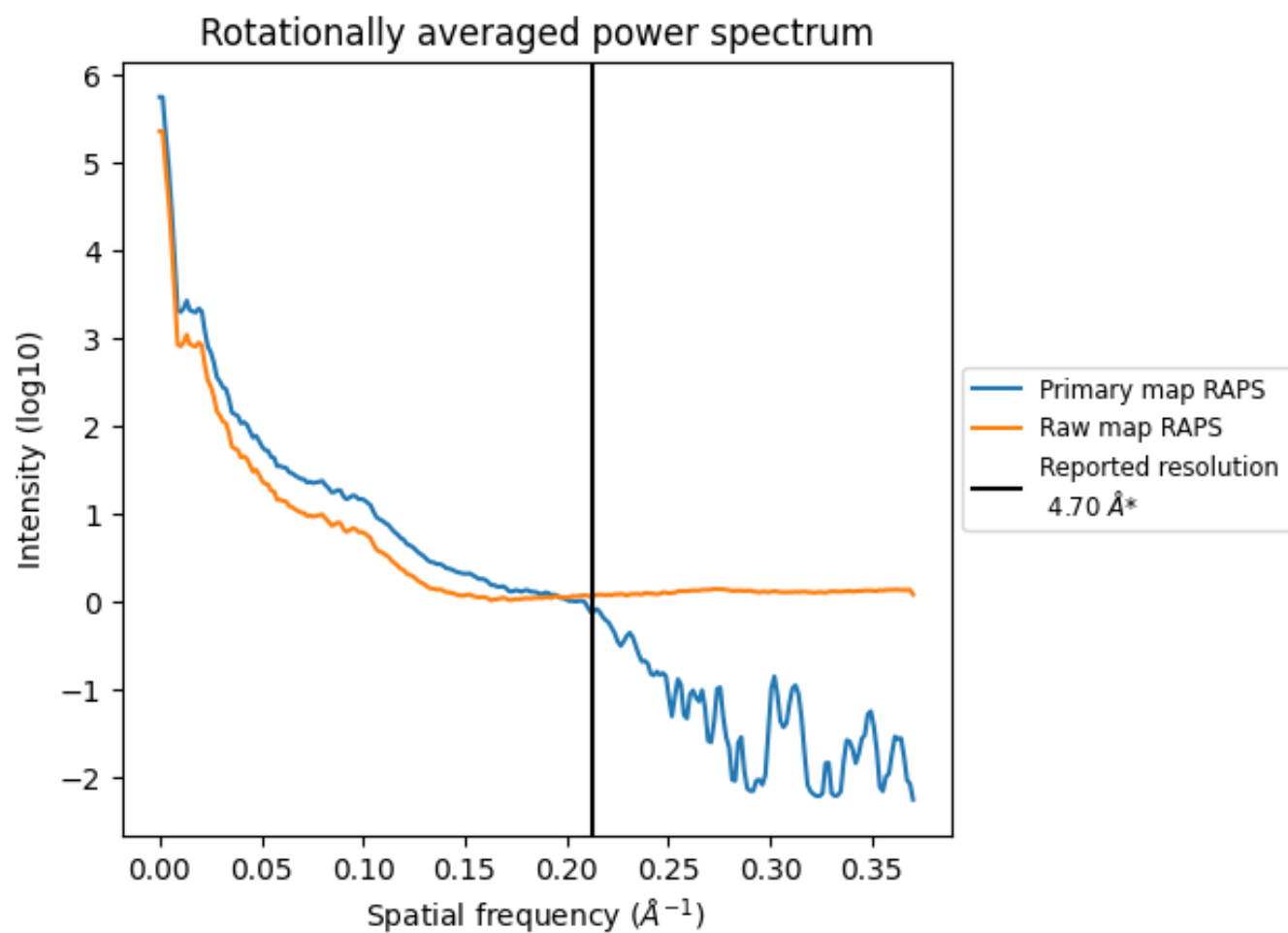
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3831 nm^3 ; this corresponds to an approximate mass of 3461 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 ⓘ

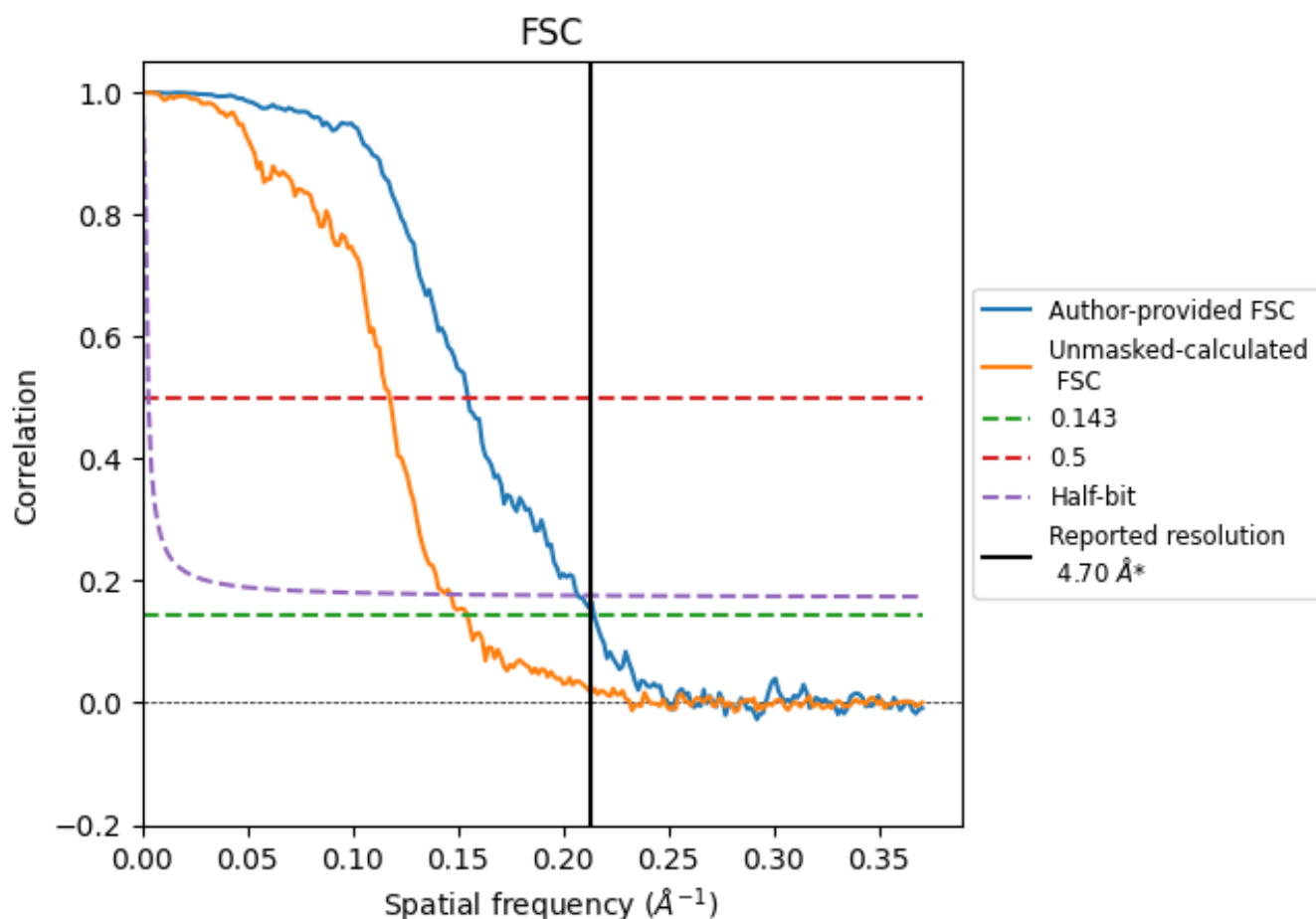


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.66	6.47	4.83
Unmasked-calculated*	6.48	8.50	6.83

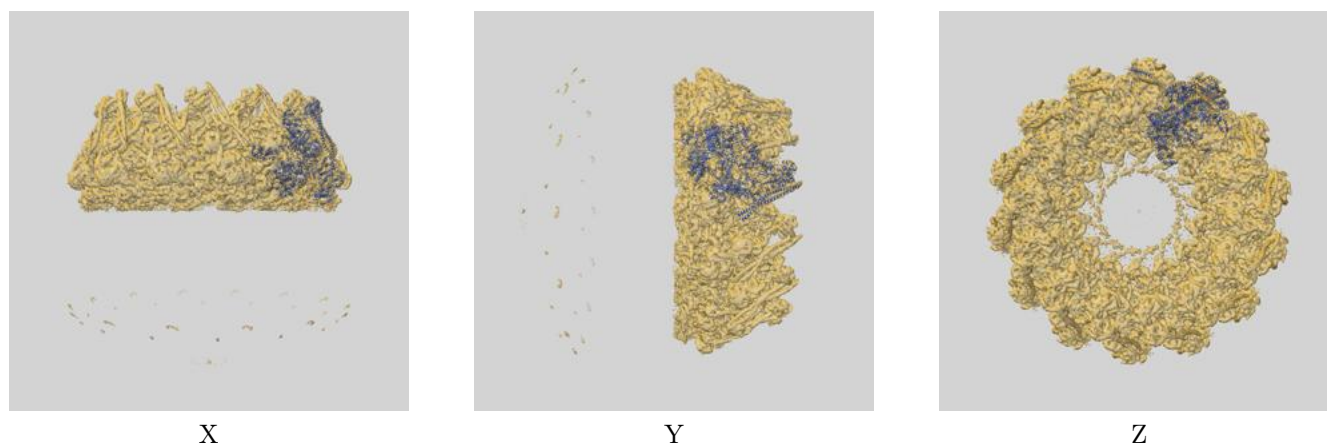
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.48 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

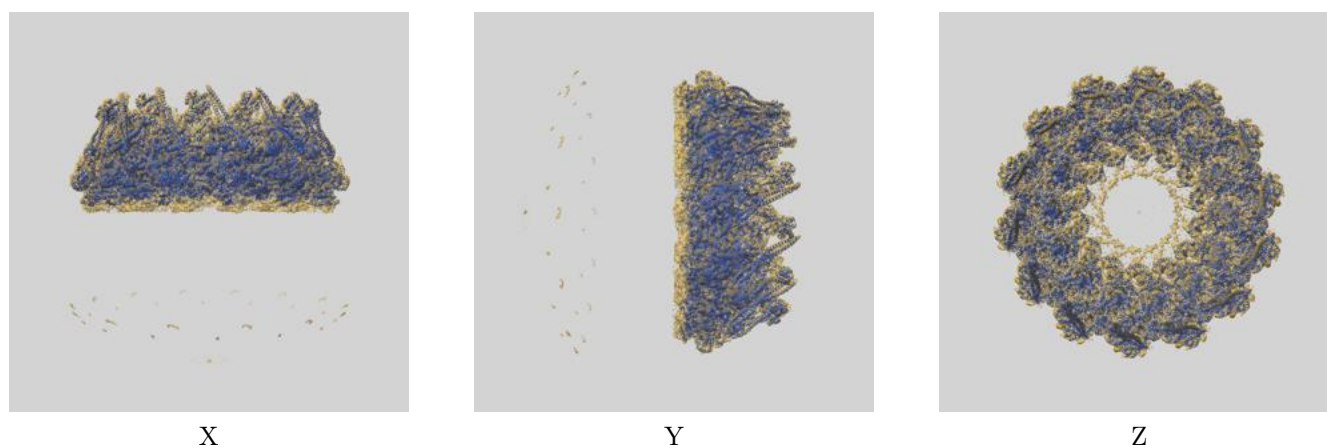
This section contains information regarding the fit between EMDB map EMD-51808 and PDB model 9H2J. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

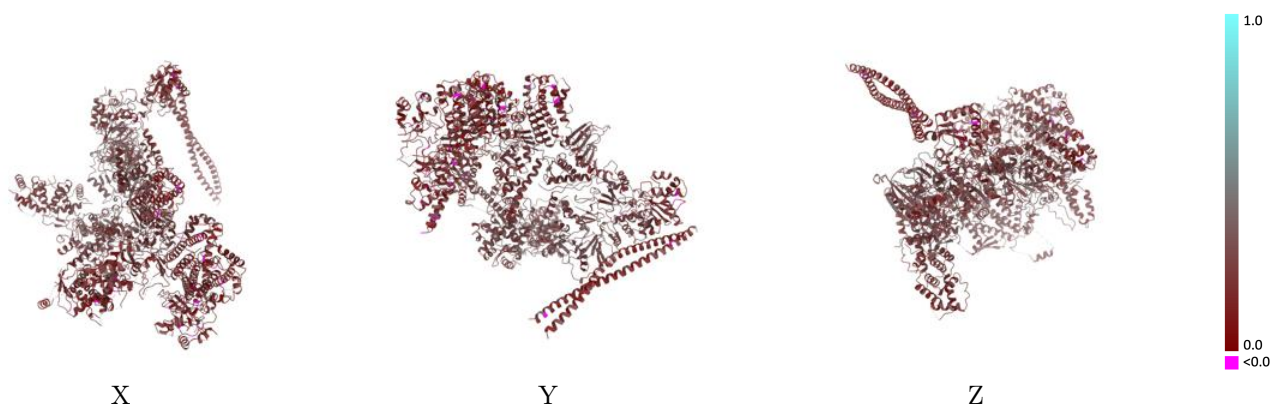


9.1.2 Map-model assembly overlay [i](#)



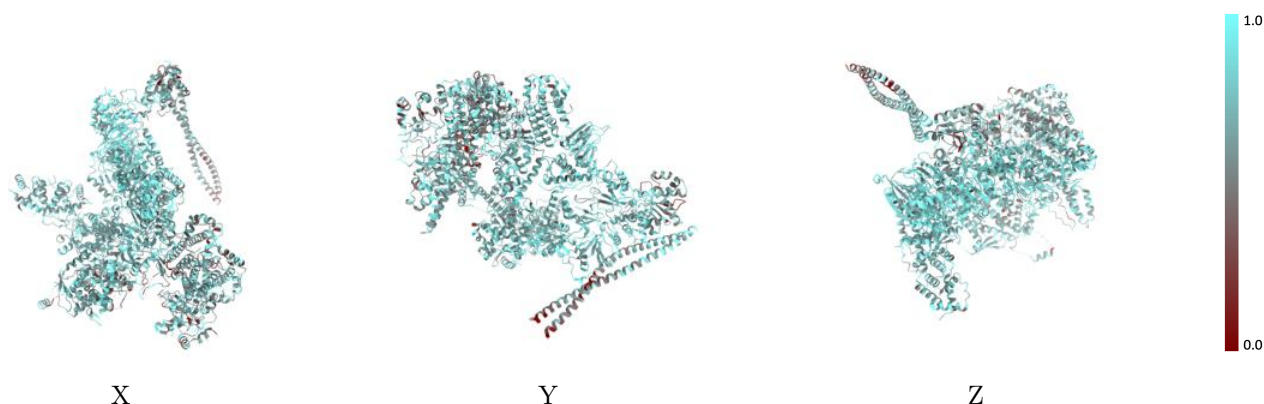
The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



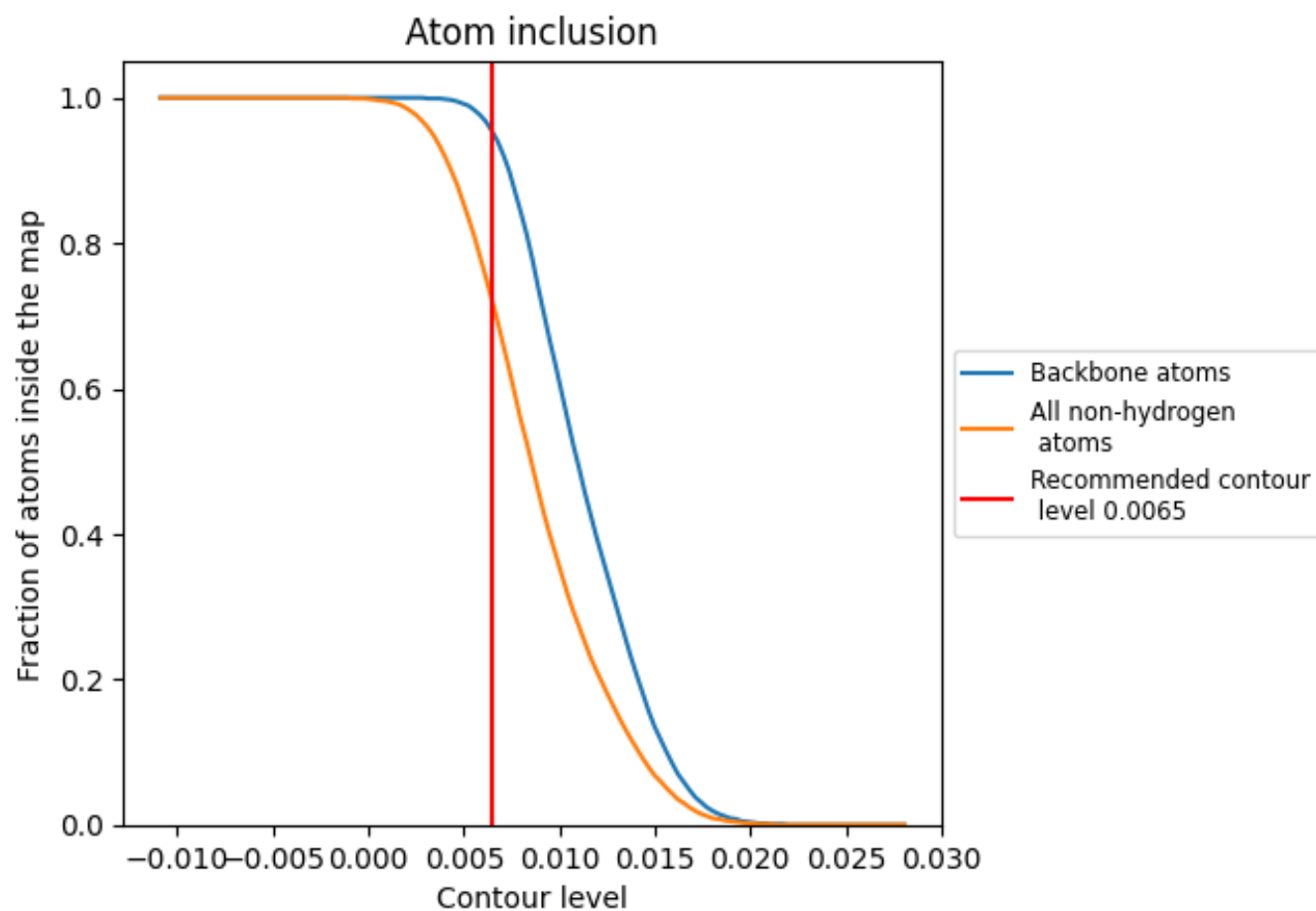
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0065).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.2570
A	 0.7360	 0.2800
B	 0.6340	 0.2120
C	 0.7800	 0.2610
D	 0.7430	 0.2370
E	 0.8100	 0.3160
F	 0.6940	 0.2060
G	 0.7220	 0.2750
H	 0.7650	 0.2320
I	 0.6180	 0.2010
J	 0.6450	 0.1970
K	 0.8210	 0.3270
L	 0.6110	 0.2080
M	 0.7050	 0.2650
N	 0.5270	 0.2000
O	 0.6140	 0.2350
P	 0.5860	 0.2130

