



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 07:00 PM JST

PDB ID : 7ETO
EMDB ID : EMD-31301
Title : C1 CVSC-binding penton vertex in the virion capsid of Human Cytomegalovirus
Authors : Li, Z.; Yu, X.
Deposited on : 2021-05-13
Resolution : 4.00 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:

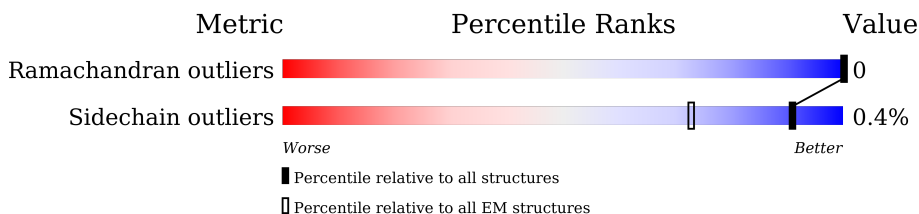
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 4.00 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	1	1048	
1	x	1048	
2	I	306	
2	h	306	
2	n	306	
2	o	306	
3	H	2241	
3	P	2241	
4	g	290	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	m	290	 9% 99%
5	M	594	 8% 78% 21%
6	N	642	 10% 90%
6	O	642	 5% 11% 89%
7	Q	75	 29% 81% 16%
7	R	75	 39% 83% 16%
7	S	75	 28% 84% 16%
7	T	75	 56% 84% 16%
7	i	75	 47% 84% 16%
7	j	75	 40% 83% 16%
8	A	1370	 16% 93% 7%
8	B	1370	 9% 97%
8	C	1370	 5% 97%
8	D	1370	 8% 94% 5%
8	Y	1370	 12% 98%
8	Z	1370	 6% 97%
8	a	1370	 6% 94% 5%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 98674 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 ORFL92C_UL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	x	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	1	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		

- Molecule 2 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	h	302	Total	C	N	O	S	0	0
			2398	1536	418	427	17		
2	I	296	Total	C	N	O	S	0	0
			2349	1506	409	417	17		
2	n	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
2	o	289	Total	C	N	O	S	0	0
			2291	1473	393	407	18		

- Molecule 3 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	20	Total	C	N	O	S	0	0
			172	110	32	29	1		
3	P	20	Total	C	N	O	S	0	0
			172	110	32	29	1		

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	g	112	Total	C	N	O	S	0	0
			929	596	164	165	4		
4	m	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 5 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	468	3848	2408	740	686	14	0	0

- Molecule 6 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	66	558	346	111	97	4	0	0
6	O	69	589	371	113	102	3	0	0

- Molecule 7 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Q	63	513	321	97	91	4	0	0
7	R	63	513	321	97	91	4	0	0
7	S	63	513	321	97	91	4	0	0
7	T	63	513	321	97	91	4	0	0
7	i	63	513	321	97	91	4	0	0
7	j	63	513	321	97	91	4	0	0

- Molecule 8 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	a	1297	10260	6526	1785	1890	59	0	0
8	A	1271	10096	6446	1746	1847	57	0	0
8	B	1335	10574	6733	1830	1950	61	0	0
8	C	1331	10549	6718	1831	1939	61	0	0
8	D	1297	10269	6538	1785	1887	59	0	0
8	Y	1347	10676	6799	1850	1966	61	0	0

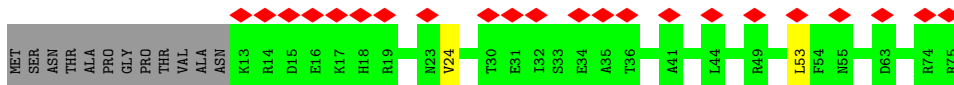
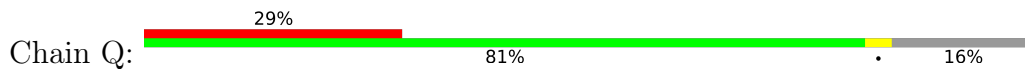
Continued on next page...

Continued from previous page...

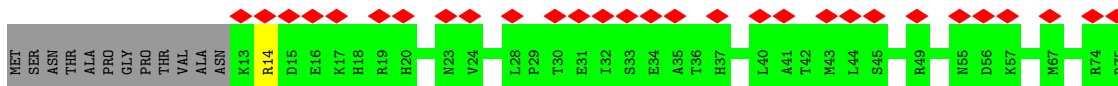
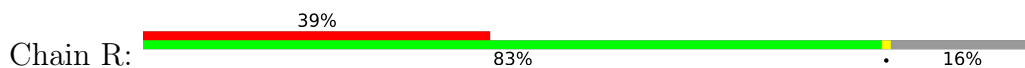
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Z	1333	10551	6720	1827	1945	59	0	0

LEU
LEU
TYR
PHE
LEU
VAL
LEU
GLY
PHE
PRO
PRO
SER
VAL
ALA
VAL
LEU

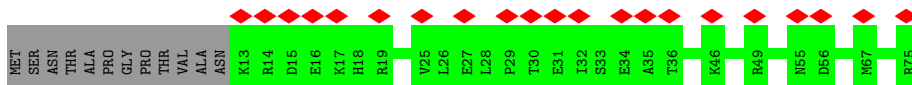
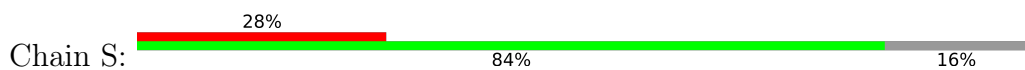
• Molecule 7: Small capsomere-interacting protein



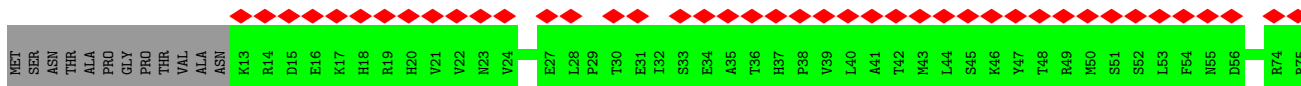
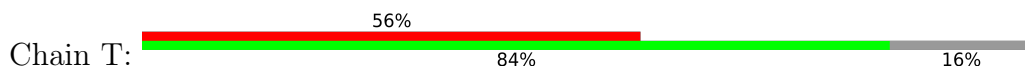
• Molecule 7: Small capsomere-interacting protein



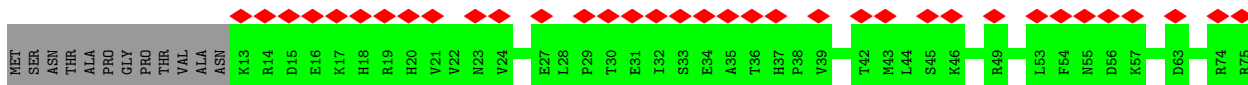
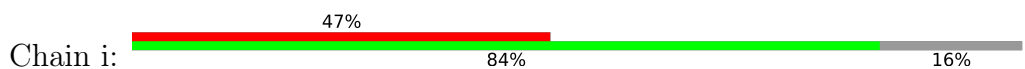
• Molecule 7: Small capsomere-interacting protein



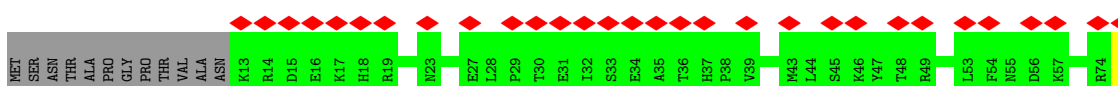
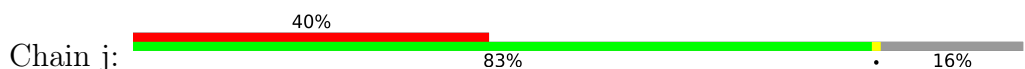
• Molecule 7: Small capsomere-interacting protein



• Molecule 7: Small capsomere-interacting protein

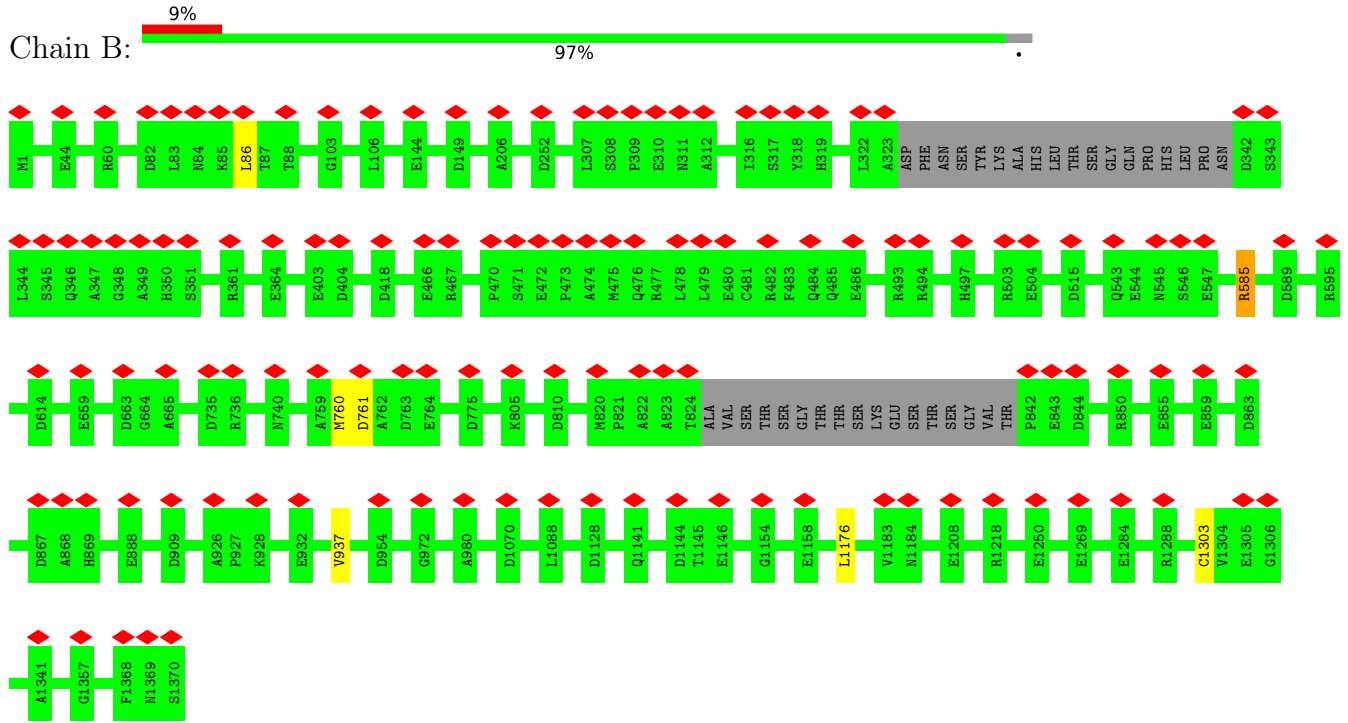


• Molecule 7: Small capsomere-interacting protein

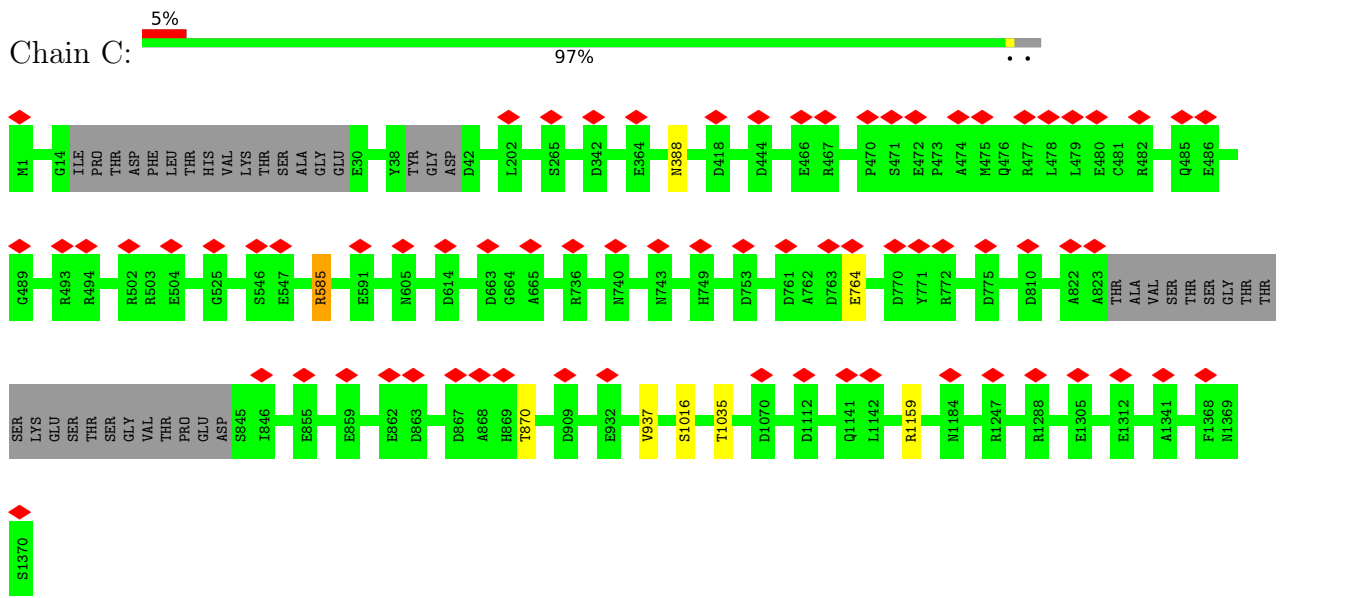


• Molecule 8: Major capsid protein

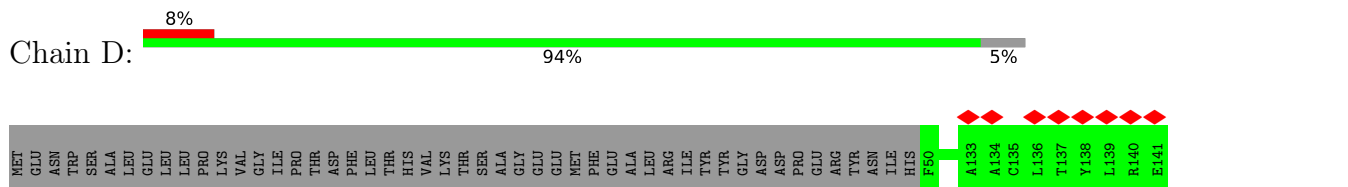
• Molecule 8: Major capsid protein

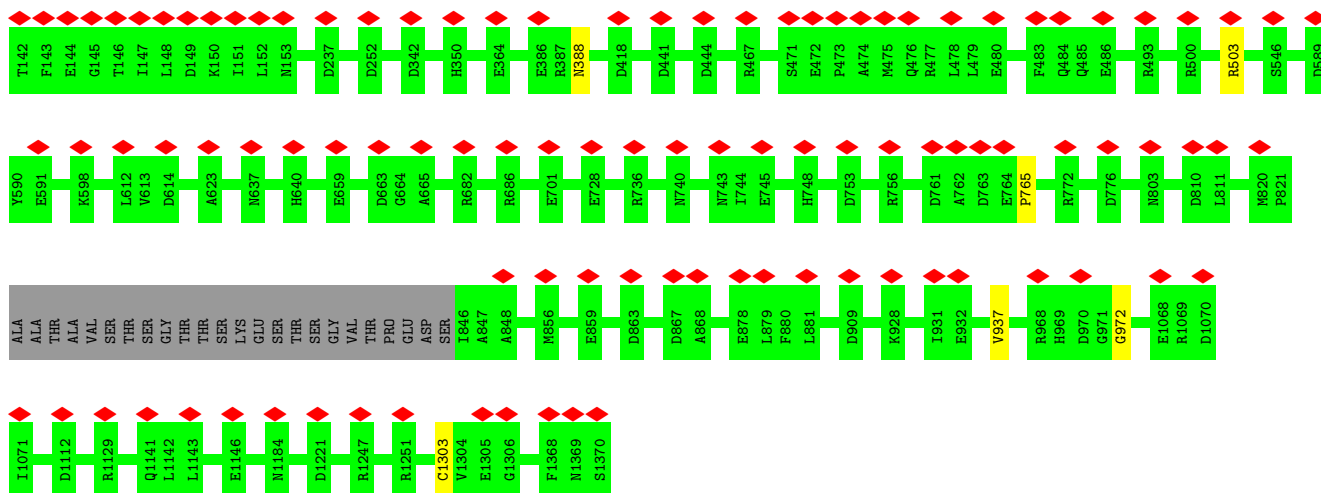


• Molecule 8: Major capsid protein

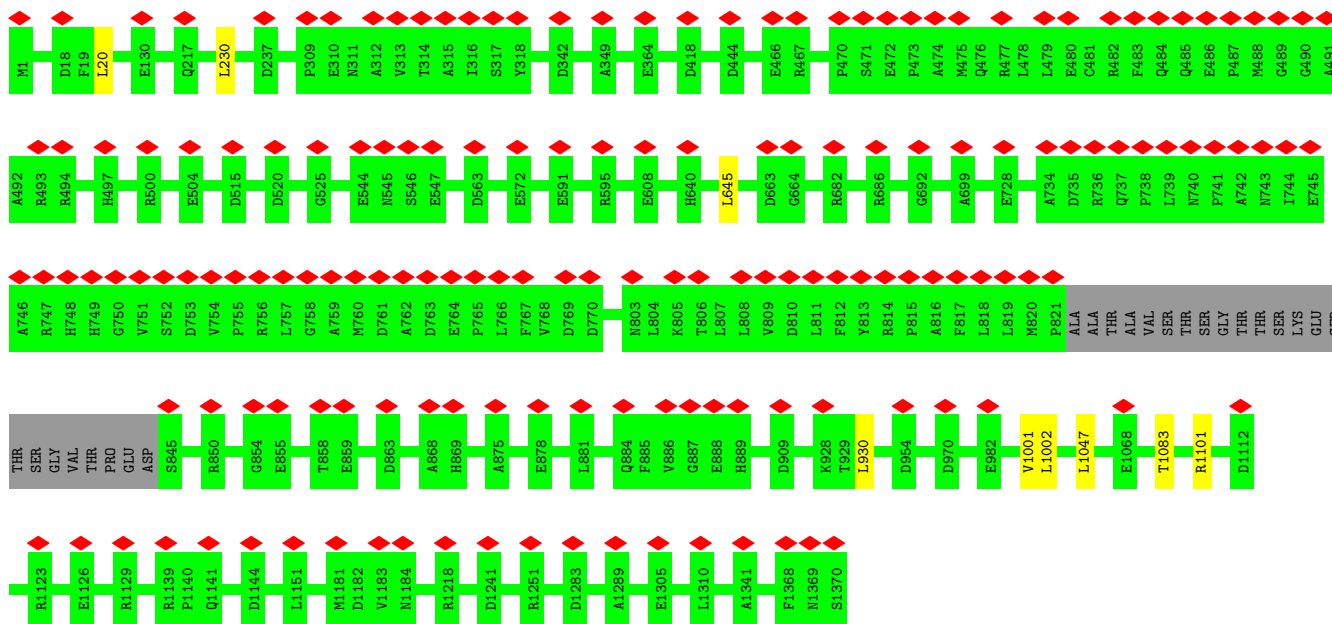


• Molecule 8: Major capsid protein

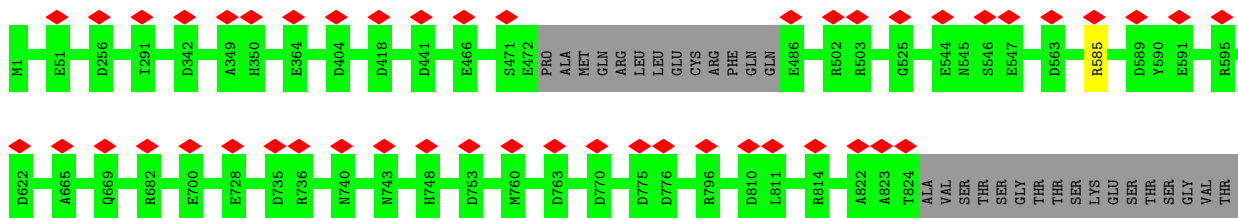


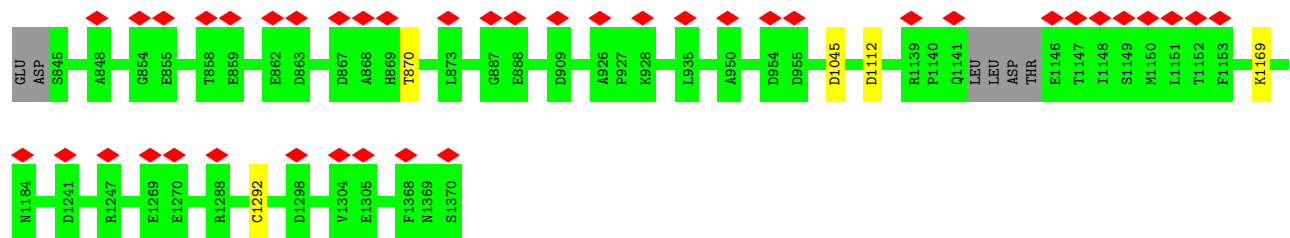


• Molecule 8: Major capsid protein



• Molecule 8: Major capsid protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131384	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.215	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.625, 1.625, 1.625	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.33	0/2366	0.58	1/3192 (0.0%)
1	x	0.35	0/2366	0.57	0/3192
2	I	0.35	0/2394	0.58	0/3251
2	h	0.37	0/2445	0.61	1/3322 (0.0%)
2	n	0.33	0/2379	0.55	0/3230
2	o	0.35	0/2333	0.54	0/3167
3	H	0.33	0/174	0.76	0/233
3	P	0.33	0/174	0.64	0/233
4	g	0.37	0/951	0.56	0/1288
4	m	0.38	0/2374	0.57	1/3221 (0.0%)
5	M	0.40	0/3935	0.56	0/5331
6	N	0.35	0/567	0.61	0/761
6	O	0.34	0/600	0.61	0/808
7	Q	0.34	0/520	0.67	1/697 (0.1%)
7	R	0.33	0/520	0.63	0/697
7	S	0.33	0/520	0.58	0/697
7	T	0.29	0/520	0.56	0/697
7	i	0.33	0/520	0.62	0/697
7	j	0.31	0/520	0.61	0/697
8	A	0.37	0/10338	0.57	1/14079 (0.0%)
8	B	0.38	0/10824	0.58	4/14743 (0.0%)
8	C	0.38	0/10799	0.56	0/14707
8	D	0.37	0/10513	0.55	0/14322
8	Y	0.36	0/10932	0.56	6/14892 (0.0%)
8	Z	0.37	0/10803	0.54	0/14716
8	a	0.39	0/10503	0.57	0/14309
All	All	0.37	0/100890	0.57	15/137179 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1
8	B	0	1
8	C	0	2
8	D	0	2
8	Z	0	1
8	a	0	2
All	All	0	9

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	761	ASP	CB-CG-OD1	8.21	125.69	118.30
1	1	184	LEU	CA-CB-CG	8.06	133.84	115.30
4	m	158	LEU	CA-CB-CG	7.71	133.02	115.30
7	Q	53	LEU	CA-CB-CG	7.15	131.75	115.30
8	Y	930	LEU	CA-CB-CG	7.04	131.48	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	B	585	ARG	Peptide
8	C	585	ARG	Peptide
2	I	250	PRO	Peptide
8	a	542	CYS	Peptide
8	a	585	ARG	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1	283/1048 (27%)	268 (95%)	15 (5%)	0	100	100
1	x	283/1048 (27%)	268 (95%)	15 (5%)	0	100	100
2	I	292/306 (95%)	279 (96%)	13 (4%)	0	100	100
2	h	300/306 (98%)	278 (93%)	22 (7%)	0	100	100
2	n	291/306 (95%)	271 (93%)	20 (7%)	0	100	100
2	o	285/306 (93%)	274 (96%)	11 (4%)	0	100	100
3	H	18/2241 (1%)	18 (100%)	0	0	100	100
3	P	18/2241 (1%)	18 (100%)	0	0	100	100
4	g	108/290 (37%)	98 (91%)	10 (9%)	0	100	100
4	m	288/290 (99%)	268 (93%)	20 (7%)	0	100	100
5	M	462/594 (78%)	424 (92%)	38 (8%)	0	100	100
6	N	64/642 (10%)	63 (98%)	1 (2%)	0	100	100
6	O	65/642 (10%)	63 (97%)	2 (3%)	0	100	100
7	Q	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	R	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
7	S	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	T	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	i	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
7	j	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
8	A	1255/1370 (92%)	1163 (93%)	92 (7%)	0	100	100
8	B	1329/1370 (97%)	1227 (92%)	102 (8%)	0	100	100
8	C	1323/1370 (97%)	1250 (94%)	73 (6%)	0	100	100
8	D	1293/1370 (94%)	1201 (93%)	92 (7%)	0	100	100
8	Y	1343/1370 (98%)	1253 (93%)	90 (7%)	0	100	100
8	Z	1325/1370 (97%)	1223 (92%)	102 (8%)	0	100	100
8	a	1293/1370 (94%)	1205 (93%)	88 (7%)	0	100	100
All	All	12284/20300 (60%)	11468 (93%)	816 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	1	256/883 (29%)	255 (100%)	1 (0%)	91	94
1	x	256/883 (29%)	254 (99%)	2 (1%)	81	89
2	I	266/273 (97%)	265 (100%)	1 (0%)	91	94
2	h	271/273 (99%)	270 (100%)	1 (0%)	91	94
2	n	263/273 (96%)	263 (100%)	0	100	100
2	o	259/273 (95%)	258 (100%)	1 (0%)	91	94
3	H	19/1941 (1%)	19 (100%)	0	100	100
3	P	19/1941 (1%)	19 (100%)	0	100	100
4	g	101/252 (40%)	101 (100%)	0	100	100
4	m	252/252 (100%)	251 (100%)	1 (0%)	91	94
5	M	395/500 (79%)	388 (98%)	7 (2%)	59	77
6	N	59/526 (11%)	59 (100%)	0	100	100
6	O	64/526 (12%)	64 (100%)	0	100	100
7	Q	59/68 (87%)	58 (98%)	1 (2%)	60	78
7	R	59/68 (87%)	58 (98%)	1 (2%)	60	78
7	S	59/68 (87%)	59 (100%)	0	100	100
7	T	59/68 (87%)	59 (100%)	0	100	100
7	i	59/68 (87%)	59 (100%)	0	100	100
7	j	59/68 (87%)	58 (98%)	1 (2%)	60	78
8	A	1109/1192 (93%)	1108 (100%)	1 (0%)	93	97
8	B	1162/1192 (98%)	1159 (100%)	3 (0%)	92	95
8	C	1159/1192 (97%)	1152 (99%)	7 (1%)	86	92
8	D	1130/1192 (95%)	1126 (100%)	4 (0%)	91	94
8	Y	1174/1192 (98%)	1171 (100%)	3 (0%)	92	95
8	Z	1159/1192 (97%)	1154 (100%)	5 (0%)	91	94
8	a	1130/1192 (95%)	1124 (100%)	6 (0%)	88	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10857/17548 (62%)	10811 (100%)	46 (0%)	91 94

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	C	585	ARG
8	D	503	ARG
8	C	870	THR
8	C	1035	THR
8	D	1303	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
8	Y	660	HIS
8	Z	1309	GLN
8	Y	1080	ASN
8	Z	660	HIS
8	a	1076	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

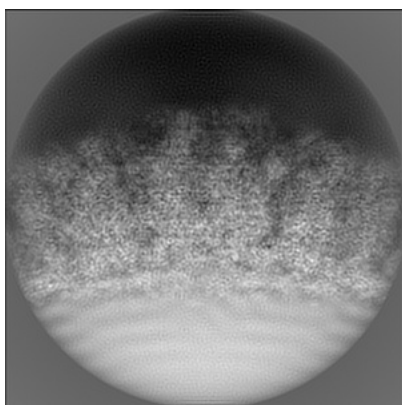
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31301. These allow visual inspection of the internal detail of the map and identification of artifacts.

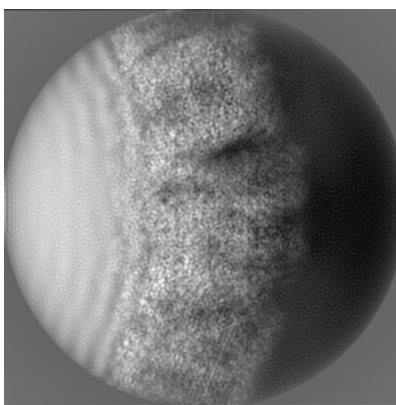
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

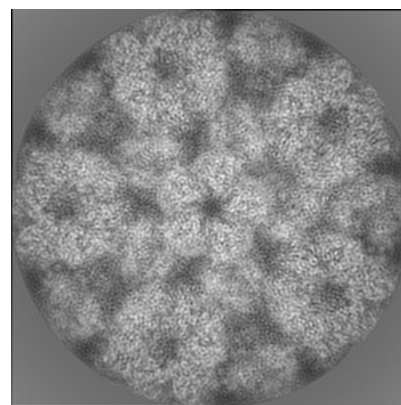
6.1.1 Primary map



X



Y

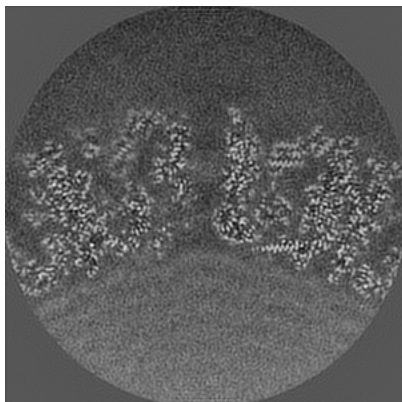


Z

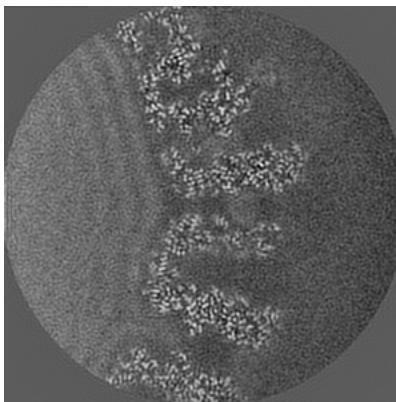
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

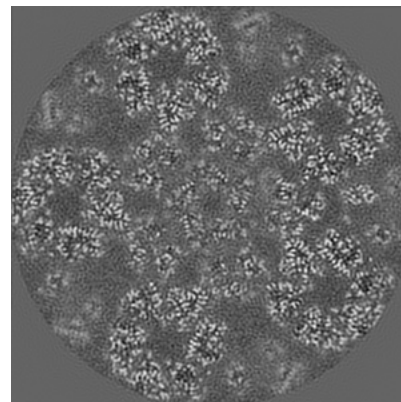
6.2.1 Primary map



X Index: 128



Y Index: 128

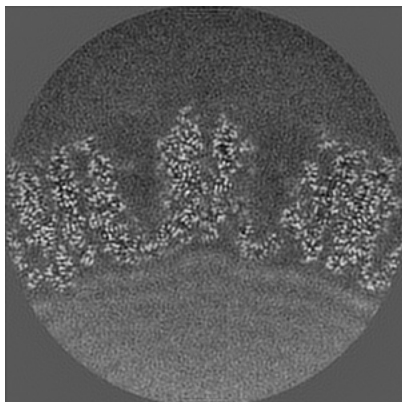


Z Index: 128

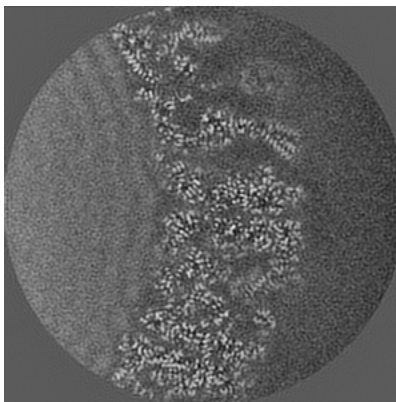
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

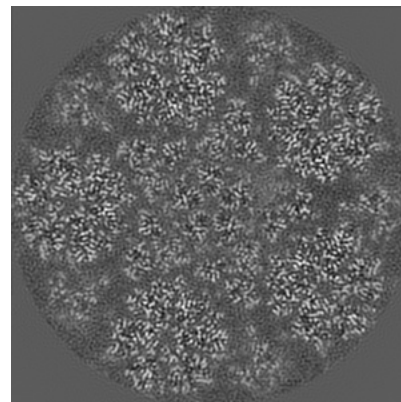
6.3.1 Primary map



X Index: 117



Y Index: 113



Z Index: 118

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

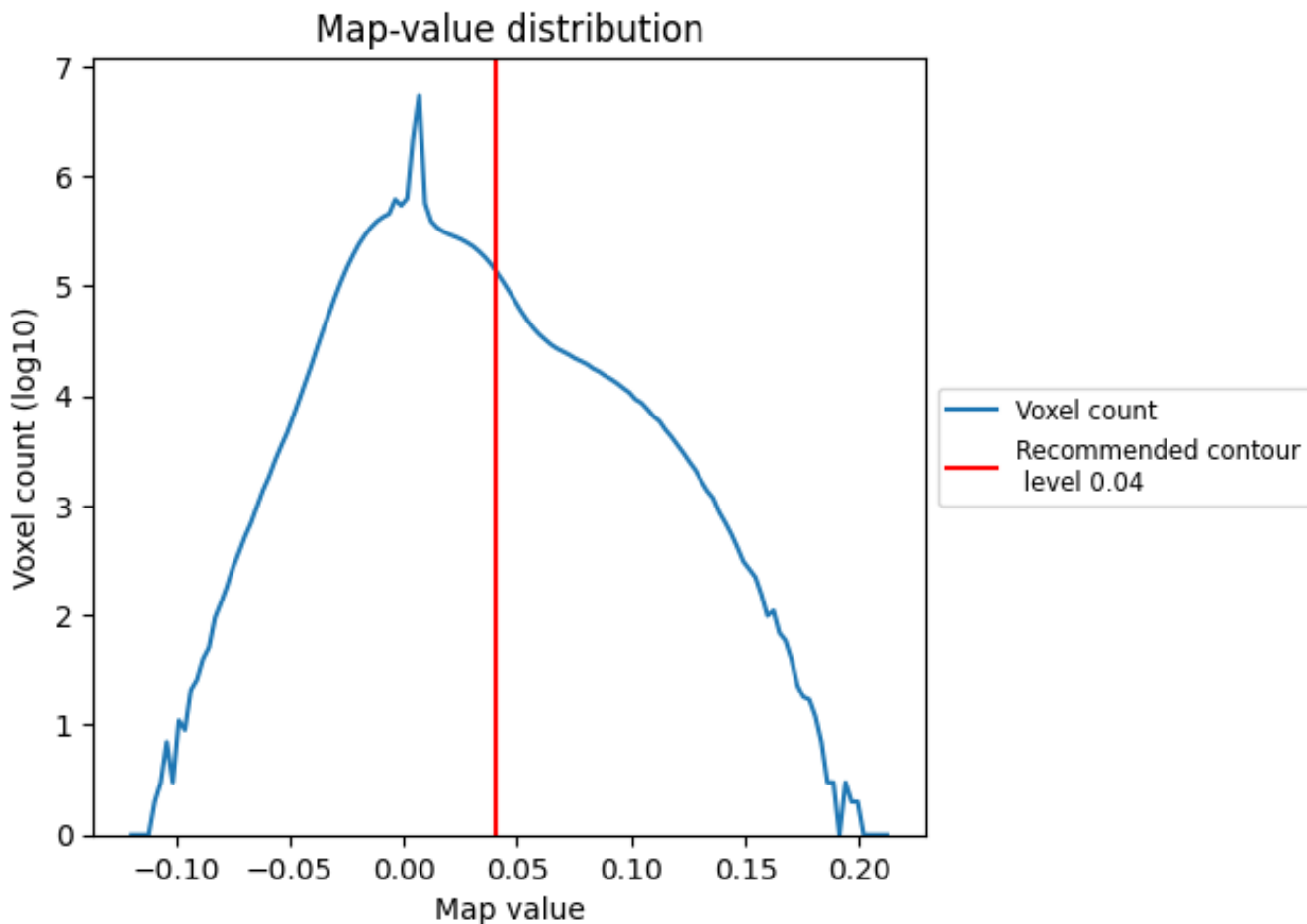
6.5 Mask visualisation

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

7 Map analysis [i](#)

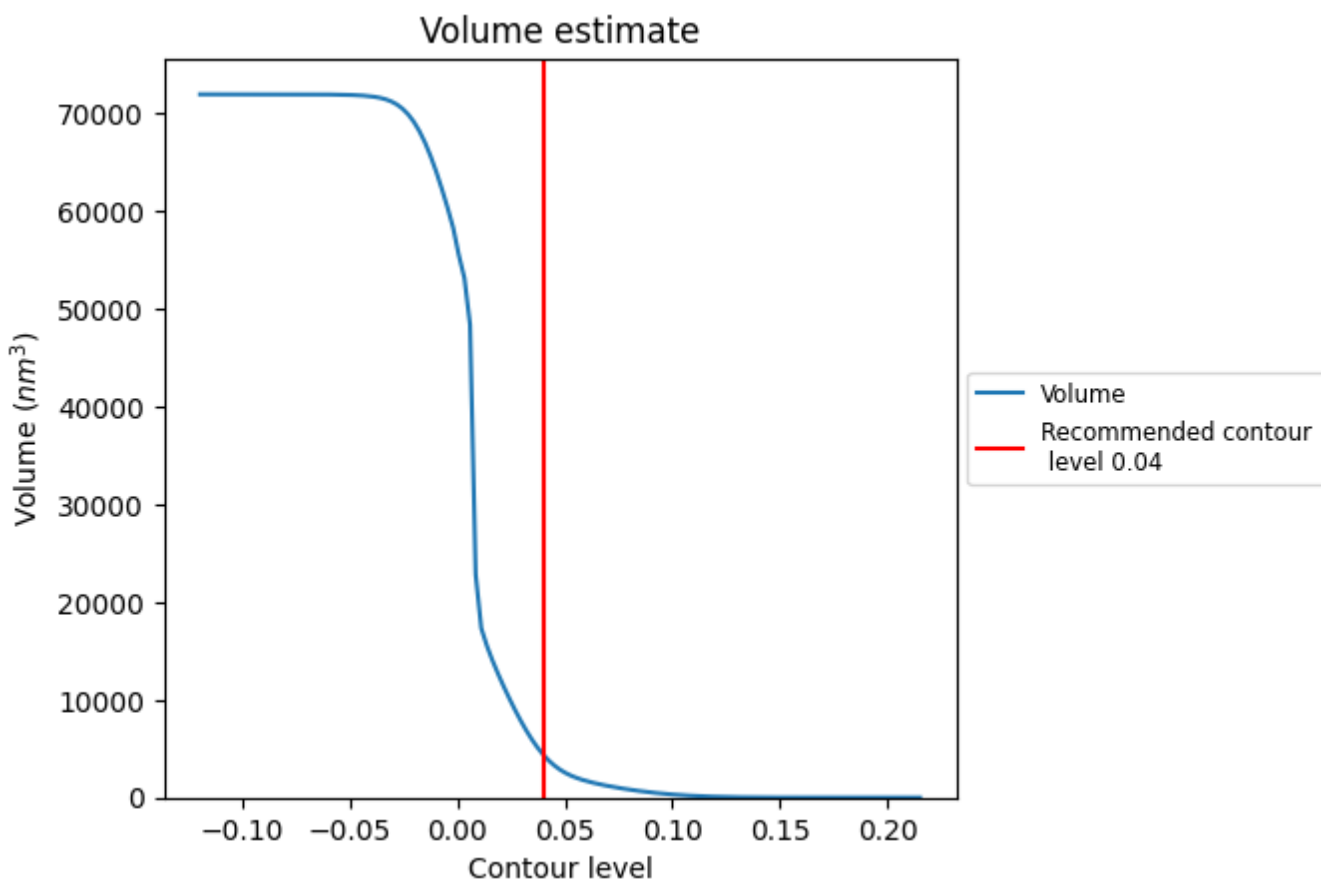
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

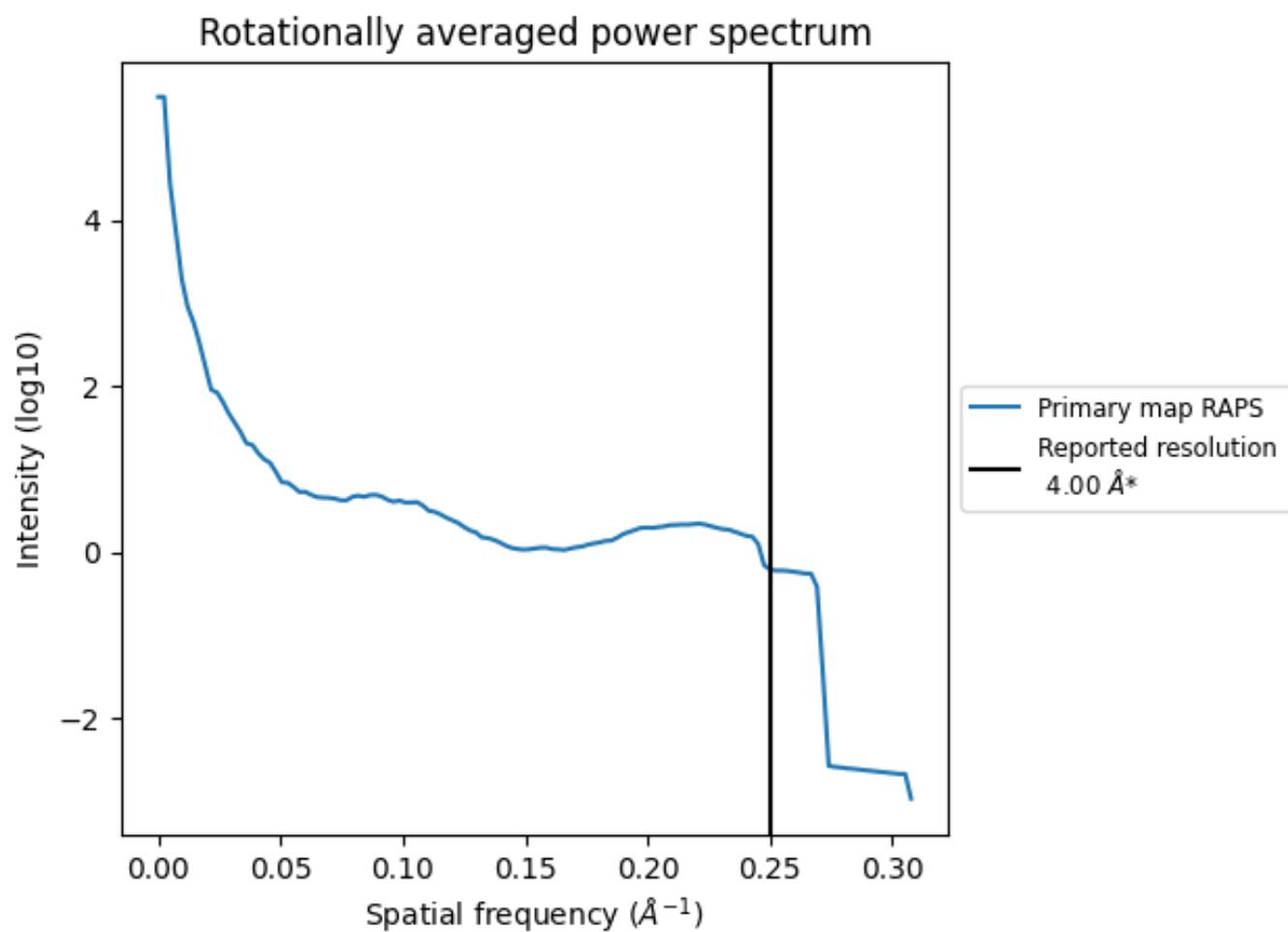
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 43822 nm³; this corresponds to an approximate mass of 3958 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 0.250 Å⁻¹

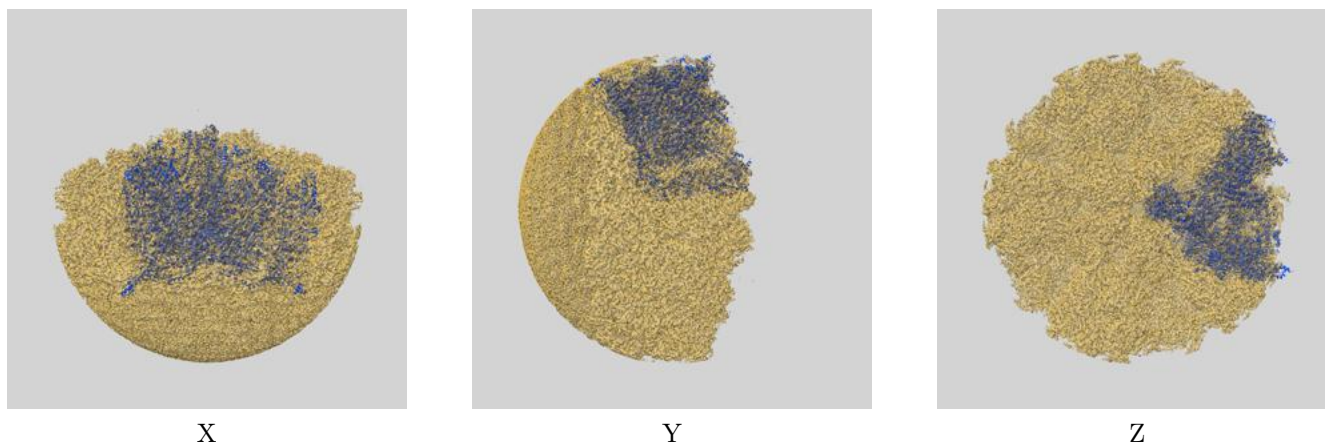
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

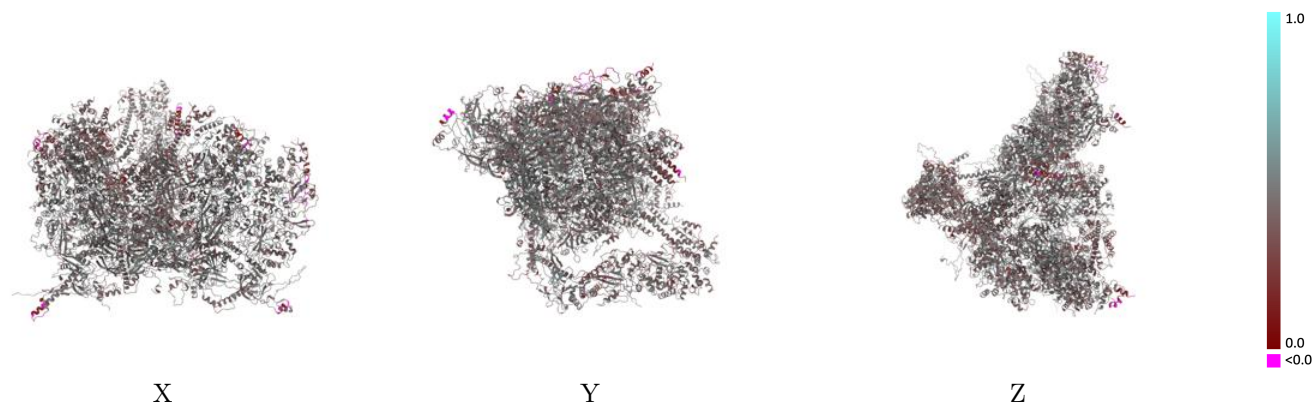
This section contains information regarding the fit between EMDB map EMD-31301 and PDB model 7ETO. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



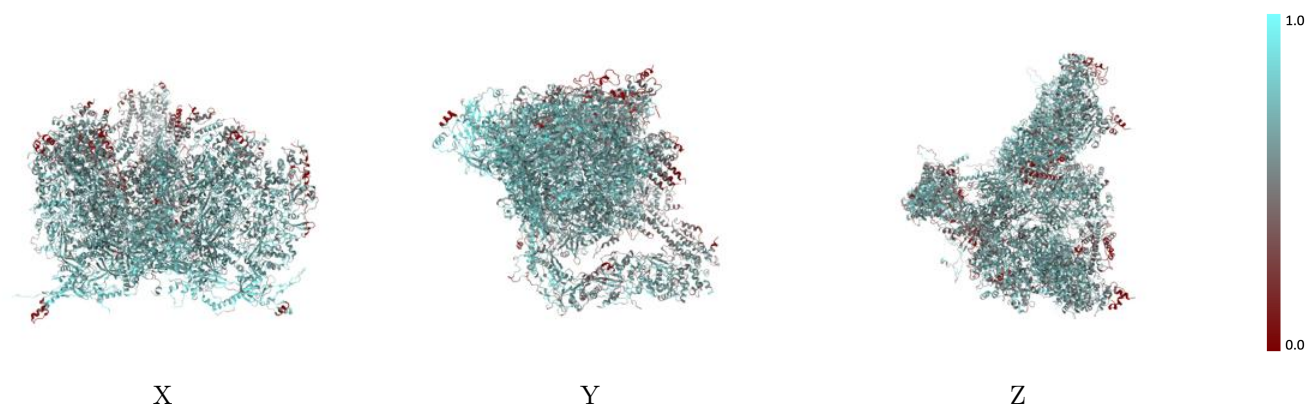
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



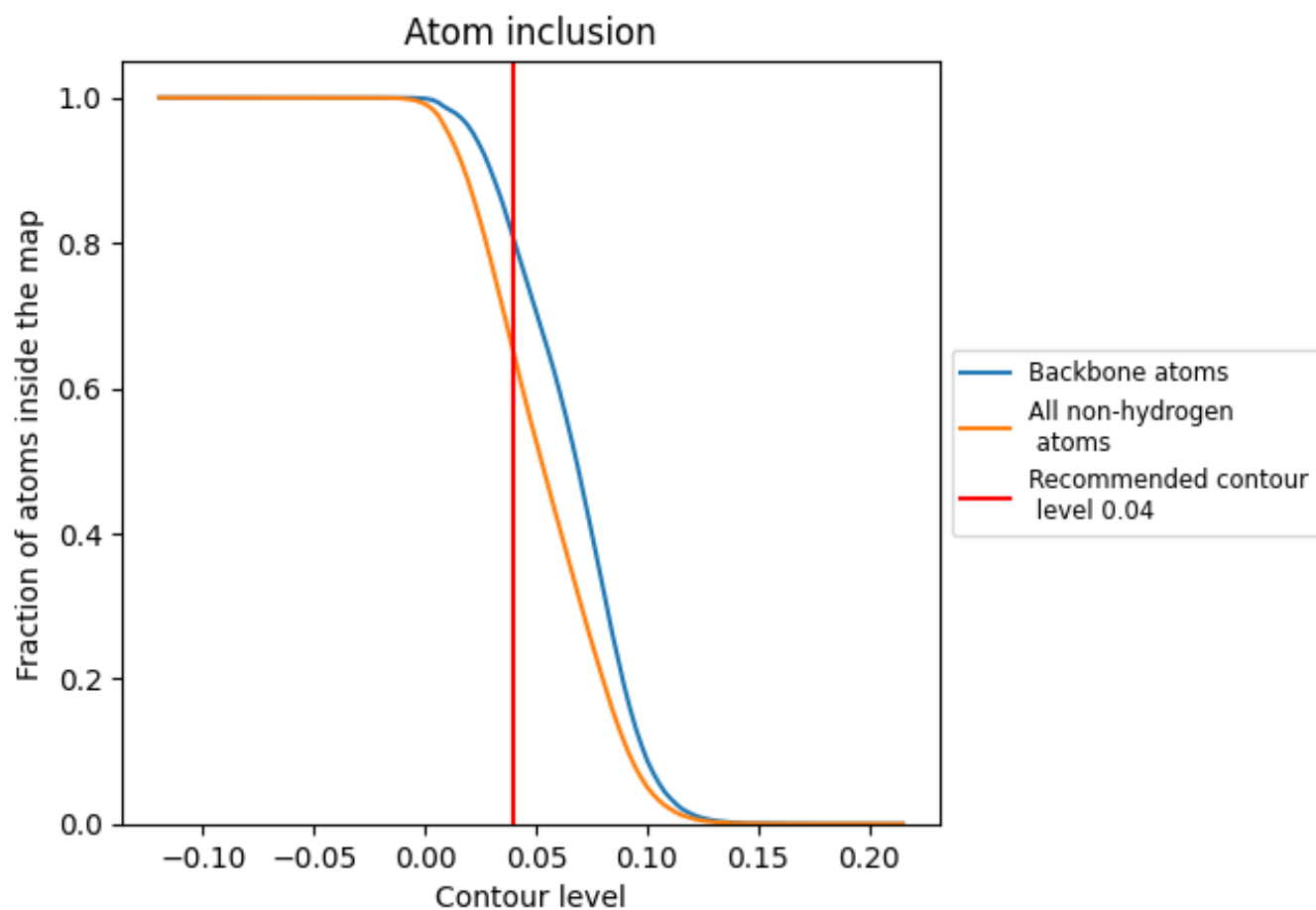
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 65% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6471	 0.4280
1	 0.4153	 0.3720
A	 0.5925	 0.4080
B	 0.6671	 0.4410
C	 0.7075	 0.4480
D	 0.6845	 0.4390
H	 0.3533	 0.3050
I	 0.5966	 0.4120
M	 0.6783	 0.4310
N	 0.5461	 0.3660
O	 0.4113	 0.2970
P	 0.3892	 0.3220
Q	 0.4598	 0.3810
R	 0.4177	 0.3790
S	 0.4739	 0.3990
T	 0.2530	 0.2750
Y	 0.6617	 0.4200
Z	 0.6916	 0.4480
a	 0.7011	 0.4510
g	 0.6250	 0.4060
h	 0.6613	 0.4150
i	 0.3273	 0.3450
j	 0.4016	 0.3890
m	 0.7066	 0.4510
n	 0.6527	 0.4190
o	 0.6505	 0.4240
x	 0.4653	 0.3860

