



## Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 02:35 AM 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

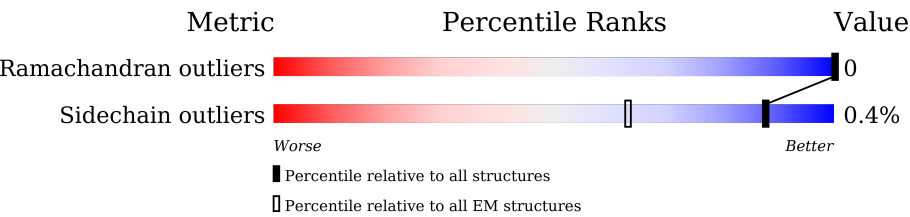
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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	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  $\geq 3$ , 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	<div><div>13%</div><div>27%</div><div>73%</div></div>
1	x	1048	<div><div>11%</div><div>27%</div><div>73%</div></div>
2	I	306	<div><div>18%</div><div>96%</div><div>..</div></div>
2	h	306	<div><div>8%</div><div>98%</div><div>..</div></div>
2	n	306	<div><div>10%</div><div>96%</div><div>.</div></div>
2	o	306	<div><div>11%</div><div>94%</div><div>6%</div></div>
3	H	2241	<div><div>.</div><div>99%</div></div>
3	P	2241	<div><div>.</div><div>99%</div></div>
4	g	290	<div><div>6%</div><div>39%</div><div>61%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	m	290	
5	M	594	
6	N	642	
6	O	642	
7	Q	75	
7	R	75	
7	S	75	
7	T	75	
7	i	75	
7	j	75	
8	A	1370	
8	B	1370	
8	C	1370	
8	D	1370	
8	Y	1370	
8	Z	1370	
8	a	1370	

## 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
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
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
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
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
5	M	468	Total	C	N	O	S	0	0
			3848	2408	740	686	14		

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

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

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

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

- Molecule 8 is a protein called Major capsid protein.

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

*Continued on next page...*

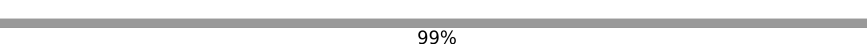
*Continued from previous page...*

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









99%

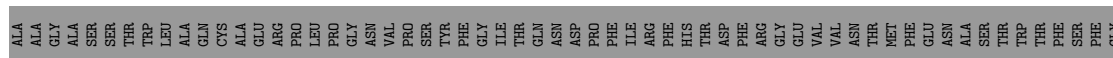
[illegible]

Diagram illustrating a 24-bit register structure, divided into 8 groups of 3 bits each. The groups are labeled L2221, R2222, Q2223, L2224, A2225, Q2226, Q2229, Q2233, H2234, M2235, L2238, Y2239, and L2240. The last group, L2240, is highlighted in grey and labeled LEU.

- Chain P:  99%



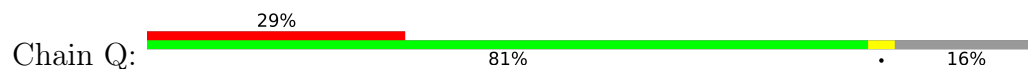






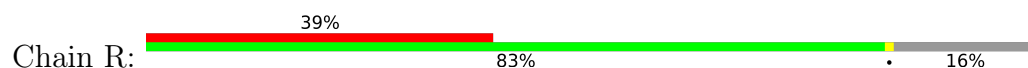
LEU  
LEU  
TYR  
PHE  
LEU  
VAL  
LEU  
GLY  
PHE  
LEU  
PRO  
SER  
VAL  
ALA  
VAL  
LEU

• Molecule 7: Small capsomere-interacting protein



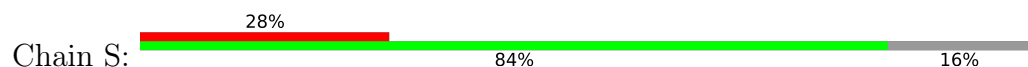
MET SER ASN THR ALA PRO GLY PRO THR VAL ALA ASN K13 R14 D15 E16 K17 H18 R19 V23 V24 T30 E31 I32 S33 E34 A35 T36 A41 L44 R49 L53 F54 N55 D63 R74 R75

• Molecule 7: Small capsomere-interacting protein



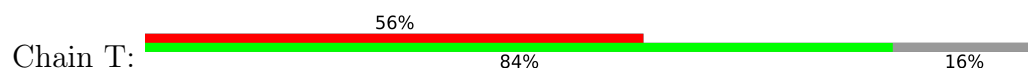
MET SER ASN THR ALA PRO GLY PRO THR VAL ALA ASN K13 R14 D15 E16 K17 H18 R19 H20 V23 V24 L28 P29 T30 E31 I32 S33 E34 A35 T36 H37 L40 A41 T42 M43 L44 S45 R49 N55 D56 K57 M67 R74 R75

• Molecule 7: Small capsomere-interacting protein



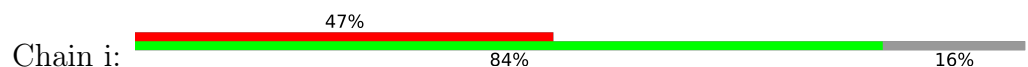
MET SER ASN THR ALA PRO GLY PRO THR VAL ALA ASN K13 R14 D15 E16 K17 H18 R19 V25 L26 E27 P29 T30 E31 I32 S33 E34 A35 T36 K46 R49 N55 D56 M57 R75

• Molecule 7: Small capsomere-interacting protein



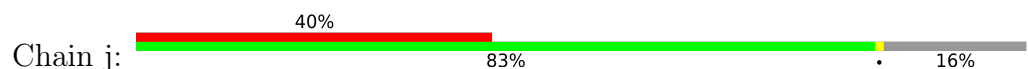
MET SER ASN THR ALA PRO GLY PRO THR VAL ALA ASN K13 R14 D15 E16 K17 H18 R19 H20 V21 V22 V23 V24 E27 L28 P29 T30 E31 I32 S33 E34 A35 T36 H37 P38 V39 L40 A41 T42 M43 L44 S45 K46 Y47 T48 R49 M50 S51 S52 L53 F54 N55 D56 R74 R75

• Molecule 7: Small capsomere-interacting protein



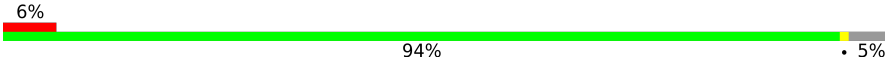
MET SER ASN THR ALA PRO GLY PRO THR VAL ALA ASN K13 R14 D15 E16 K17 H18 R19 H20 V21 V22 V23 V24 E27 L28 P29 T30 E31 I32 S33 E34 A35 T36 H37 P38 V39 T42 M43 L44 S45 K46 R49 L53 F54 N55 D56 K57 D63 R74 R75

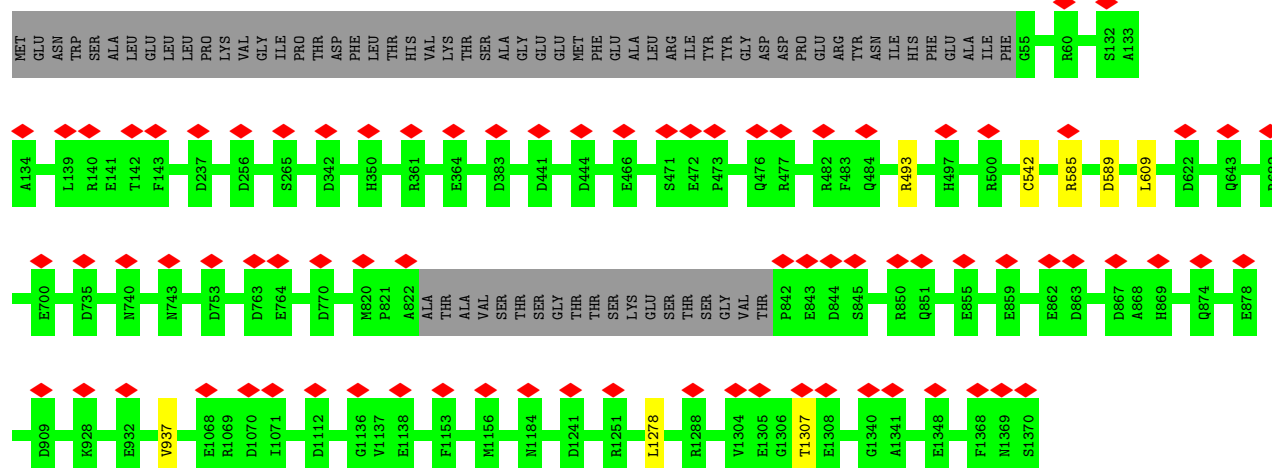
• Molecule 7: Small capsomere-interacting protein



MET SER ASN THR ALA PRO GLY PRO THR VAL ALA ASN K13 R14 D15 E16 K17 H18 R19 V23 L28 P29 T30 E31 I32 S33 E34 A35 T36 H37 P38 V39 M43 L44 S45 Y47 T48 R49 L53 F54 N55 D56 K57 R74 R75

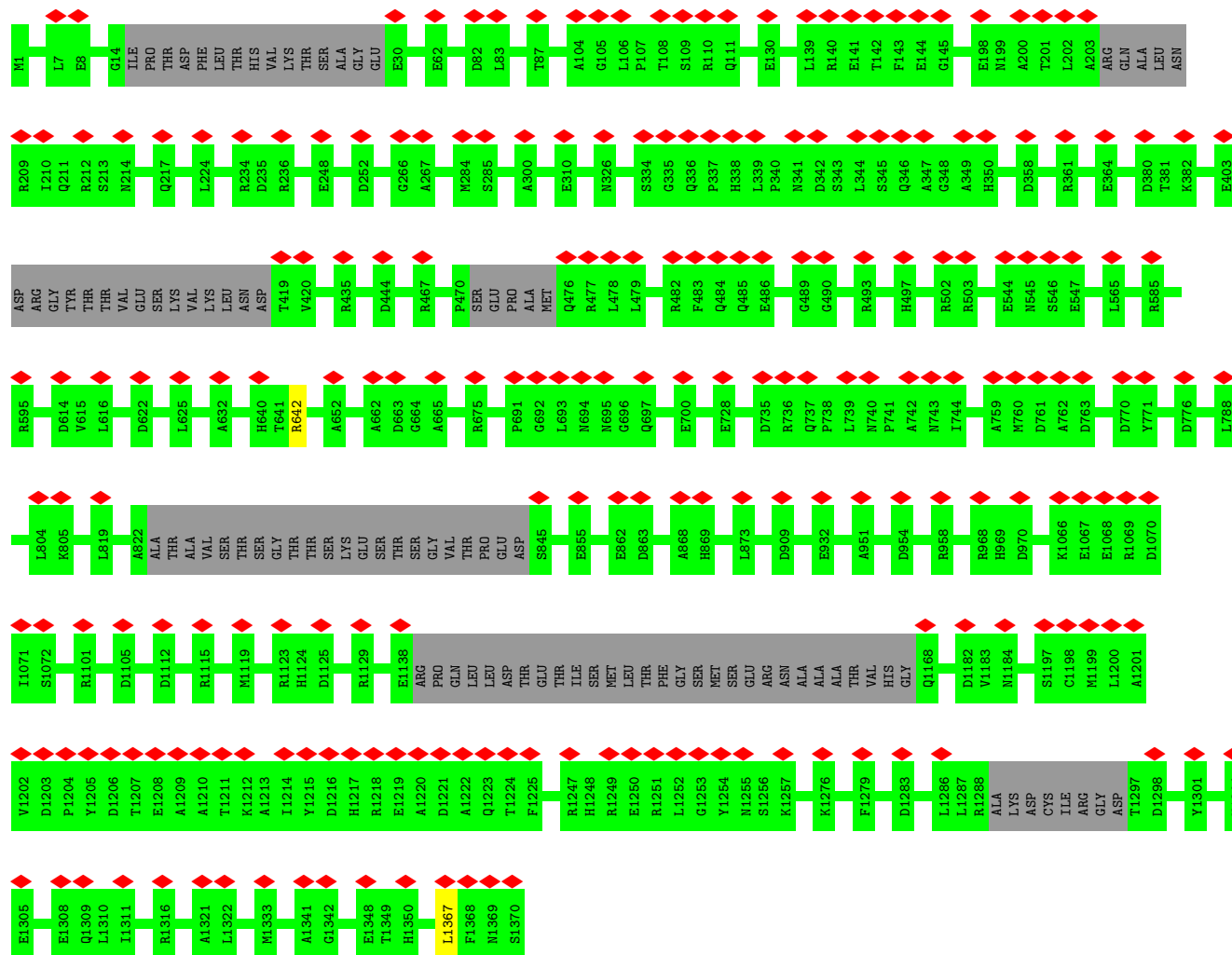
• Molecule 8: Major capsid protein

Chain a:  6% 94% 5%

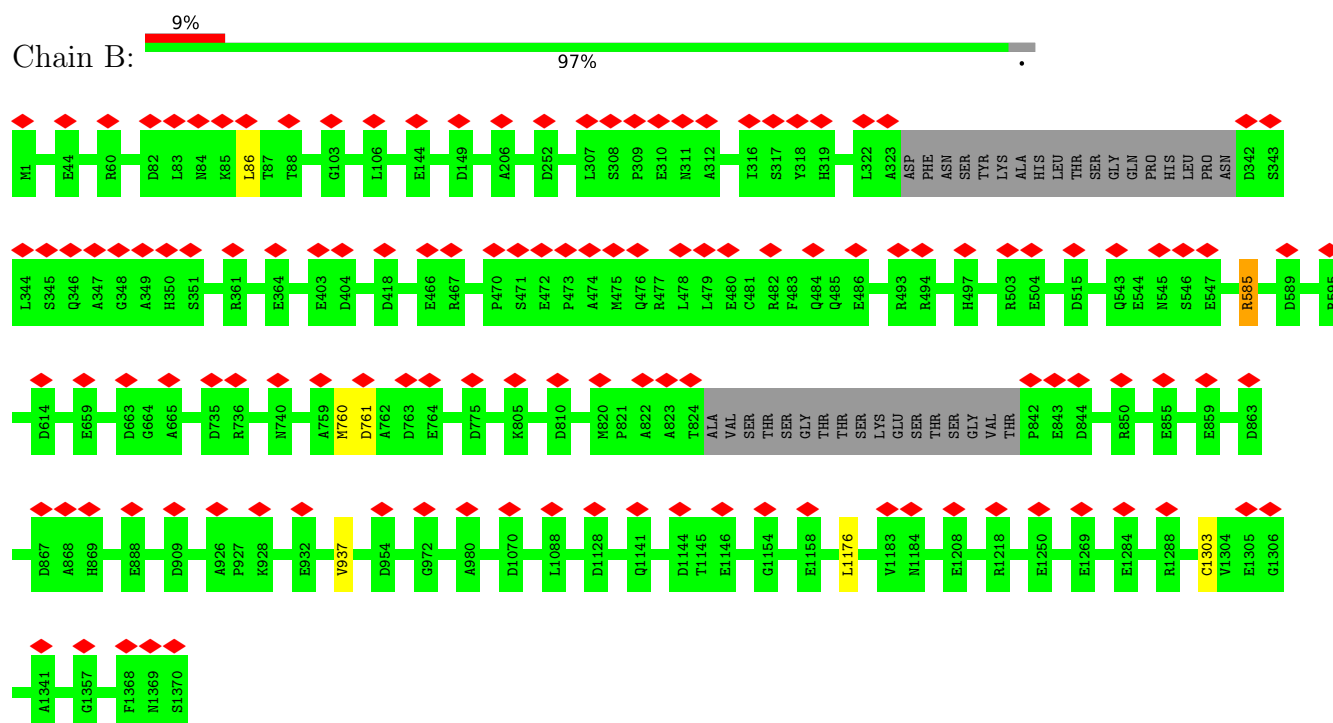


• Molecule 8: Major capsid protein

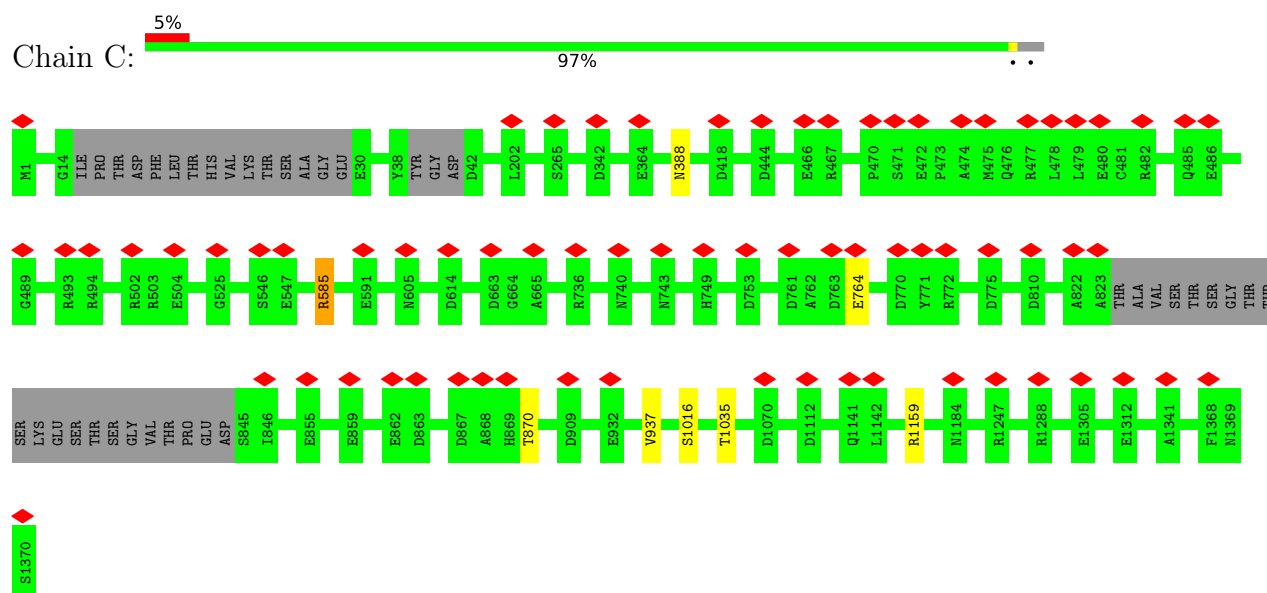
Chain A:  16% 93% 7%



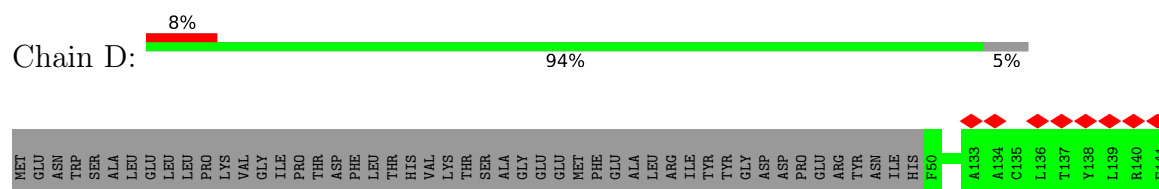
- Molecule 8: Major capsid protein

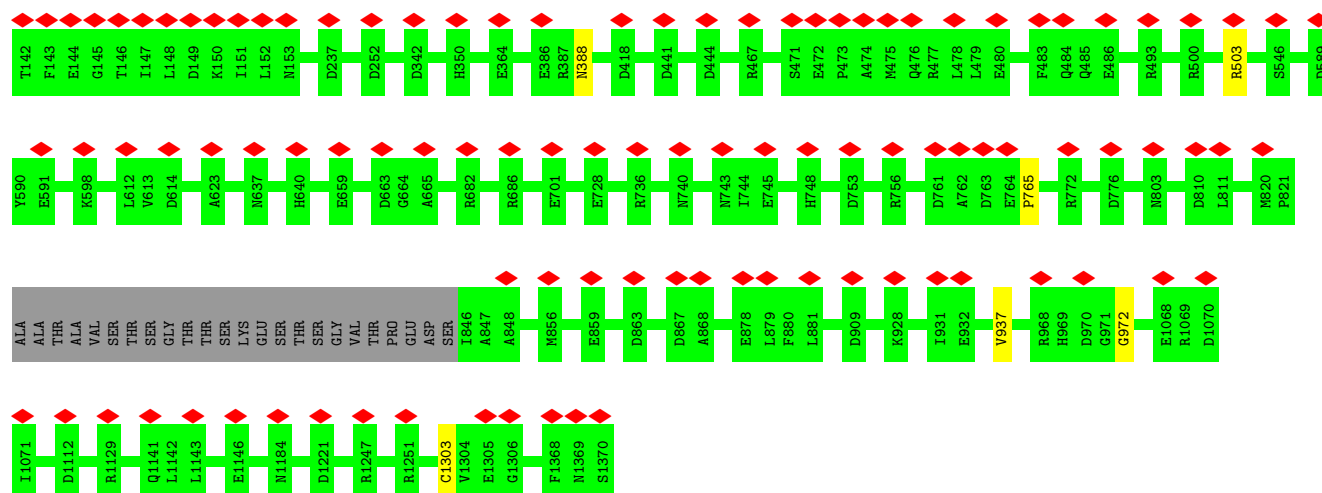


- Molecule 8: Major capsid protein

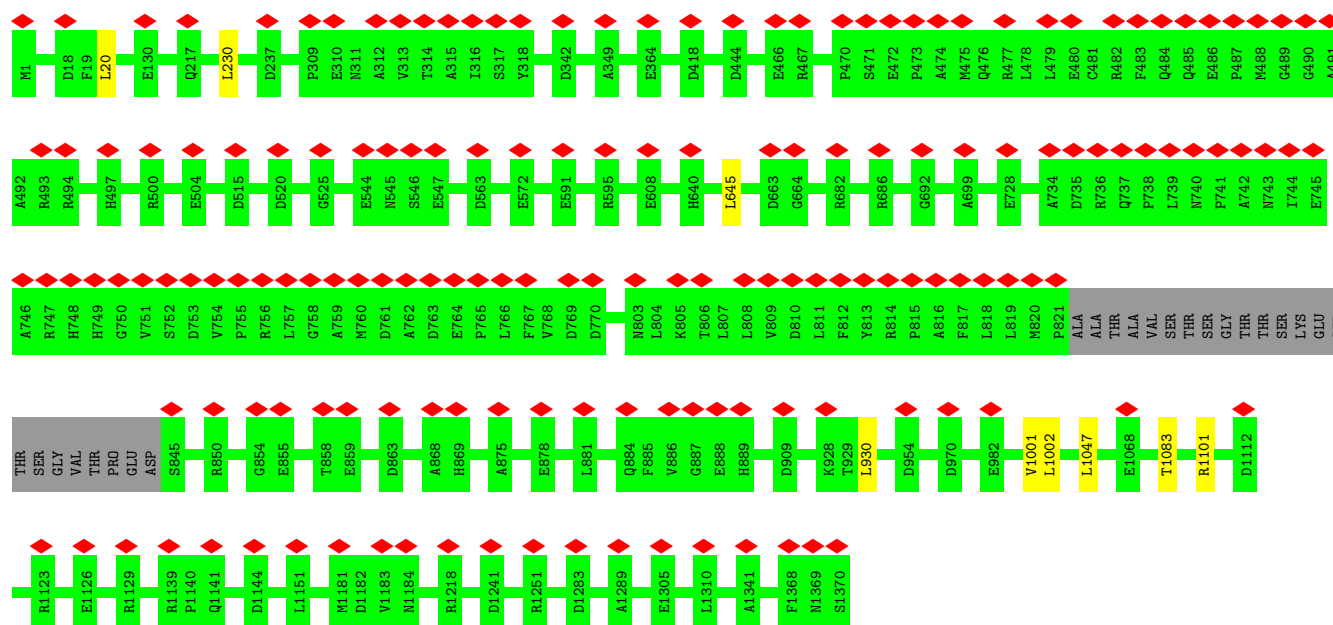


- Molecule 8: Major capsid protein

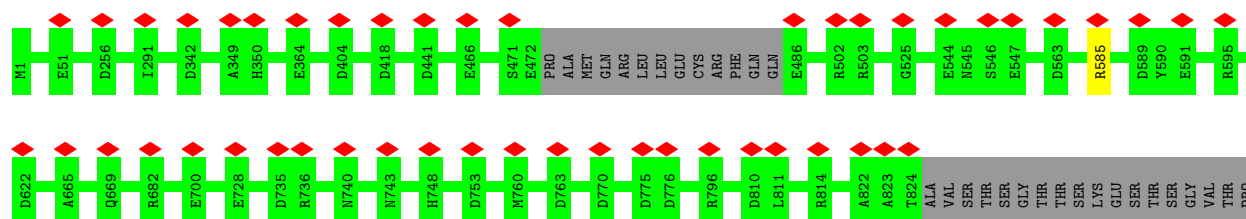


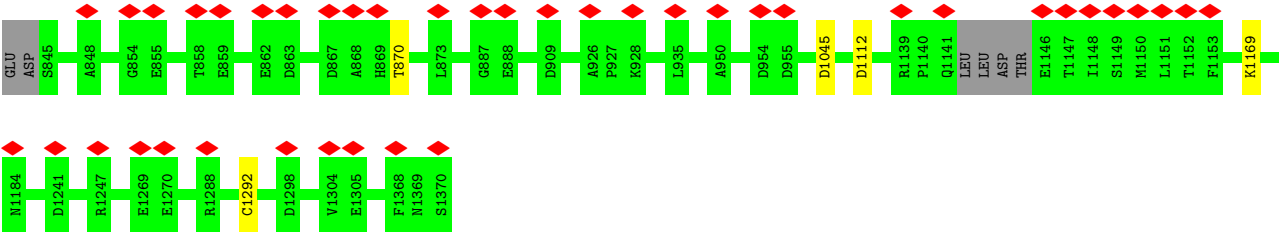


• Molecule 8: Major capsid protein



• 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

### 5.1 Standard geometry

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	l	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.

All (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	l	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
8	B	86	LEU	CA-CB-CG	6.85	131.06	115.30
8	B	1176	LEU	CA-CB-CG	6.25	129.68	115.30
8	Y	20	LEU	CA-CB-CG	6.10	129.34	115.30
2	h	124	LEU	CA-CB-CG	5.92	128.92	115.30
8	Y	1002	LEU	CA-CB-CG	5.64	128.28	115.30
8	Y	645	LEU	CA-CB-CG	5.27	127.43	115.30
8	B	760	MET	C-N-CA	5.22	134.75	121.70
8	Y	1047	LEU	CA-CB-CG	5.20	127.26	115.30
8	Y	230	LEU	CA-CB-CG	5.17	127.19	115.30
8	A	1367	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	B	585	ARG	Peptide
8	C	585	ARG	Peptide
8	C	764	GLU	Peptide
8	D	765	PRO	Peptide
8	D	972	GLY	Peptide
2	I	250	PRO	Peptide
8	Z	585	ARG	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	89	91
1	x	256/883 (29%)	254 (99%)	2 (1%)	79	84
2	I	266/273 (97%)	265 (100%)	1 (0%)	89	91
2	h	271/273 (99%)	270 (100%)	1 (0%)	89	91
2	n	263/273 (96%)	263 (100%)	0	100	100
2	o	259/273 (95%)	258 (100%)	1 (0%)	89	91
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%)	89	91
5	M	395/500 (79%)	388 (98%)	7 (2%)	54	71
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%)	56	72
7	R	59/68 (87%)	58 (98%)	1 (2%)	56	72
7	S	59/68 (87%)	59 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	56	72
8	A	1109/1192 (93%)	1108 (100%)	1 (0%)	92	94
8	B	1162/1192 (98%)	1159 (100%)	3 (0%)	91	92
8	C	1159/1192 (97%)	1152 (99%)	7 (1%)	84	88
8	D	1130/1192 (95%)	1126 (100%)	4 (0%)	89	91
8	Y	1174/1192 (98%)	1171 (100%)	3 (0%)	91	92
8	Z	1159/1192 (97%)	1154 (100%)	5 (0%)	89	91
8	a	1130/1192 (95%)	1124 (100%)	6 (0%)	86	89
All	All	10857/17548 (62%)	10811 (100%)	46 (0%)	88	91

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	10	ARG
1	x	258	VAL
2	h	121	ARG
2	I	255	ARG
2	o	241	LEU
4	m	35	VAL
5	M	44	TYR
5	M	76	VAL
5	M	84	ARG
5	M	113	THR
5	M	131	THR
5	M	163	PHE
5	M	164	LEU
1	1	44	LYS
7	Q	24	VAL
7	R	14	ARG
7	j	75	ARG
8	a	493	ARG
8	a	589	ASP
8	a	609	LEU
8	a	937	VAL
8	a	1278	LEU
8	a	1307	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	A	642	ARG
8	B	585	ARG
8	B	937	VAL
8	B	1303	CYS
8	C	388	ASN
8	C	585	ARG
8	C	870	THR
8	C	937	VAL
8	C	1016	SER
8	C	1035	THR
8	C	1159	ARG
8	D	388	ASN
8	D	503	ARG
8	D	937	VAL
8	D	1303	CYS
8	Y	1001	VAL
8	Y	1083	THR
8	Y	1101	ARG
8	Z	870	THR
8	Z	1045	ASP
8	Z	1112	ASP
8	Z	1169	LYS
8	Z	1292	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	x	34	HIS
1	x	170	ASN
1	x	198	ASN
1	x	201	ASN
2	h	84	HIS
2	h	209	ASN
2	h	235	GLN
2	I	14	HIS
2	I	50	GLN
2	I	170	GLN
2	I	257	GLN
3	P	2233	GLN
2	n	14	HIS
2	n	79	ASN
2	n	80	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	n	116	HIS
2	n	277	GLN
2	n	297	ASN
2	o	88	HIS
2	o	147	ASN
2	o	297	ASN
4	g	213	GLN
4	m	40	HIS
4	m	183	GLN
4	m	240	GLN
5	M	34	ASN
5	M	120	GLN
5	M	333	ASN
5	M	463	ASN
5	M	561	ASN
6	O	63	GLN
1	1	4	GLN
1	1	158	HIS
7	Q	37	HIS
7	T	55	ASN
7	i	37	HIS
8	a	338	HIS
8	a	510	ASN
8	a	514	GLN
8	a	534	HIS
8	a	618	HIS
8	a	737	GLN
8	a	749	HIS
8	a	794	ASN
8	a	795	ASN
8	a	945	ASN
8	a	1000	ASN
8	a	1023	GLN
8	a	1076	HIS
8	a	1245	ASN
8	a	1248	HIS
8	a	1264	GLN
8	a	1267	ASN
8	a	1313	ASN
8	A	278	ASN
8	A	510	ASN
8	A	534	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	A	581	HIS
8	A	618	HIS
8	A	676	ASN
8	A	967	HIS
8	A	1023	GLN
8	A	1076	HIS
8	A	1191	ASN
8	A	1235	GLN
8	A	1369	ASN
8	B	214	ASN
8	B	346	GLN
8	B	350	HIS
8	B	485	GLN
8	B	497	HIS
8	B	510	ASN
8	B	514	GLN
8	B	534	HIS
8	B	560	ASN
8	B	694	ASN
8	B	874	GLN
8	B	940	HIS
8	B	1229	HIS
8	C	510	ASN
8	C	514	GLN
8	C	534	HIS
8	C	676	ASN
8	C	726	ASN
8	C	849	GLN
8	C	851	GLN
8	C	903	GLN
8	C	914	GLN
8	C	919	ASN
8	C	1184	ASN
8	C	1191	ASN
8	C	1229	HIS
8	C	1255	ASN
8	D	290	HIS
8	D	371	ASN
8	D	438	GLN
8	D	476	GLN
8	D	514	GLN
8	D	534	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	D	914	GLN
8	D	965	HIS
8	D	981	HIS
8	D	1023	GLN
8	D	1080	ASN
8	D	1191	ASN
8	D	1350	HIS
8	Y	22	HIS
8	Y	76	HIS
8	Y	84	ASN
8	Y	231	ASN
8	Y	326	ASN
8	Y	432	ASN
8	Y	510	ASN
8	Y	534	HIS
8	Y	560	ASN
8	Y	660	HIS
8	Y	794	ASN
8	Y	914	GLN
8	Y	1029	HIS
8	Y	1080	ASN
8	Y	1093	ASN
8	Y	1229	HIS
8	Y	1230	ASN
8	Y	1264	GLN
8	Y	1300	GLN
8	Y	1313	ASN
8	Y	1369	ASN
8	Z	49	HIS
8	Z	111	GLN
8	Z	618	HIS
8	Z	660	HIS
8	Z	676	ASN
8	Z	795	ASN
8	Z	849	GLN
8	Z	874	GLN
8	Z	905	GLN
8	Z	1060	ASN
8	Z	1061	ASN
8	Z	1082	ASN
8	Z	1166	HIS
8	Z	1168	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	Z	1230	ASN
8	Z	1235	GLN
8	Z	1309	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

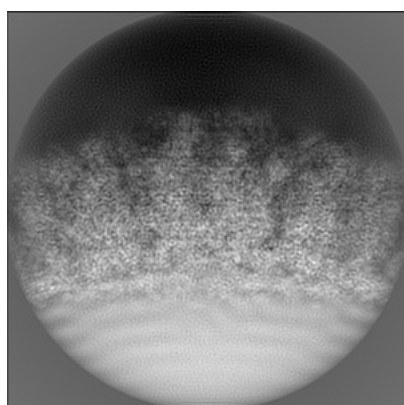
## 6 Map visualisation [i](#)

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.

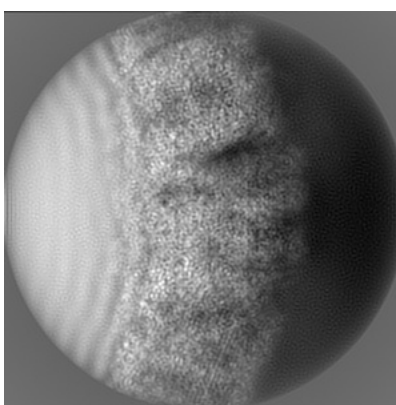
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

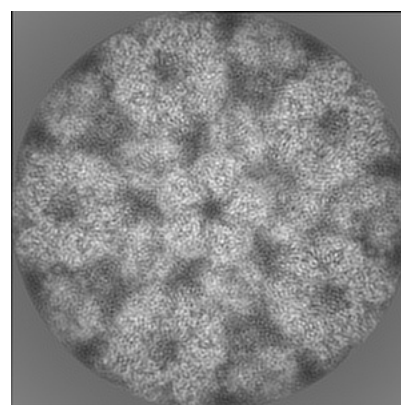
#### 6.1.1 Primary map



X



Y

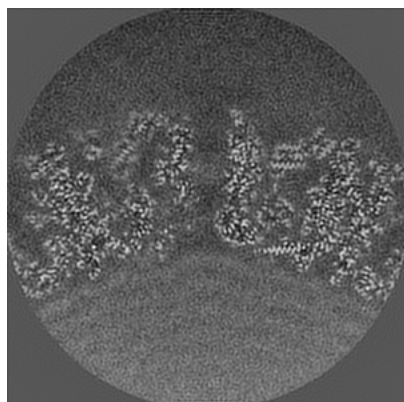


Z

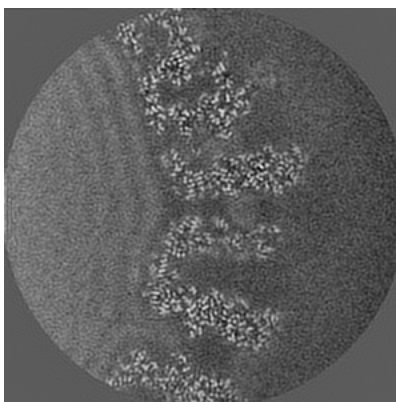
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

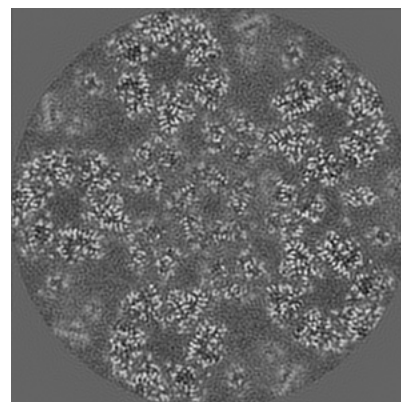
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

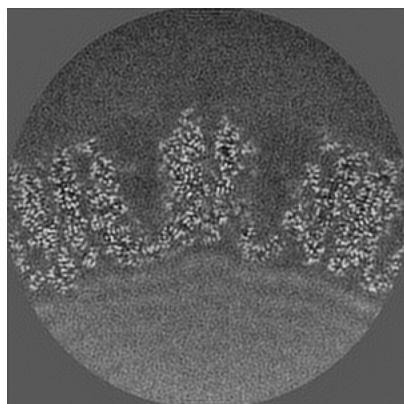


Z Index: 128

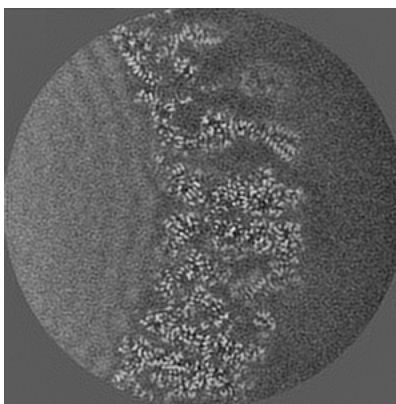
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

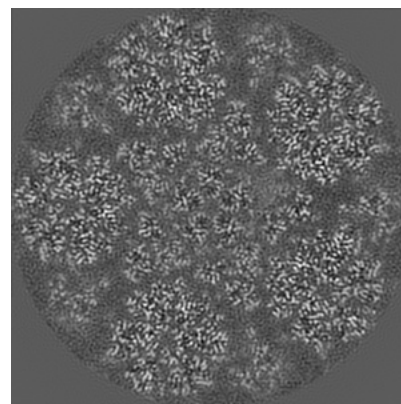
### 6.3.1 Primary map



X Index: 117



Y Index: 113

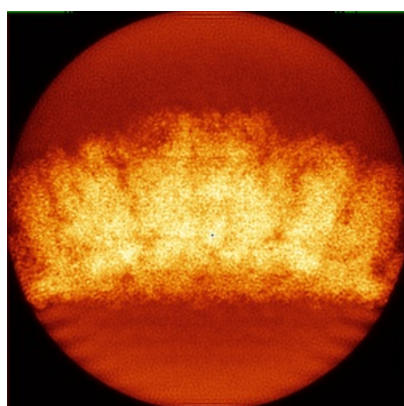


Z Index: 118

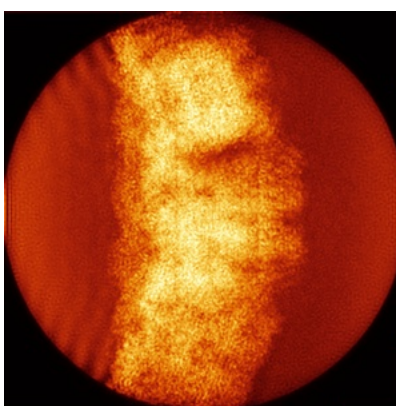
The images above show the largest variance slices of the map in three orthogonal directions.

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

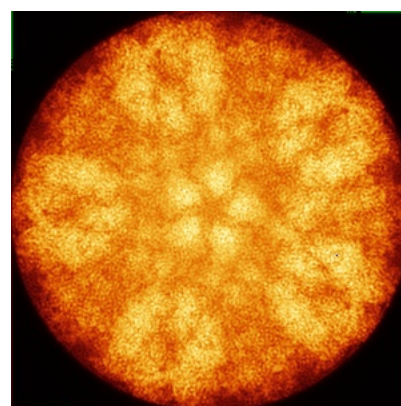
### 6.4.1 Primary map



X



Y

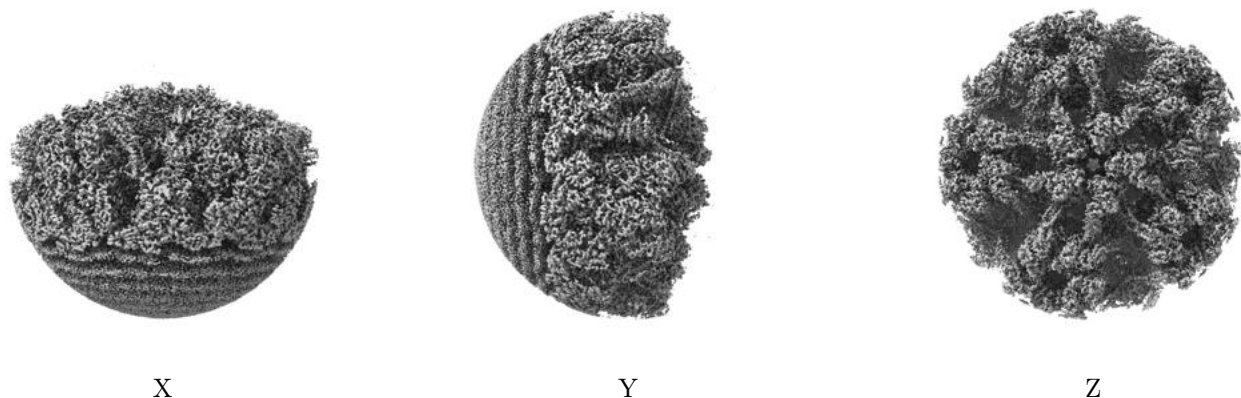


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

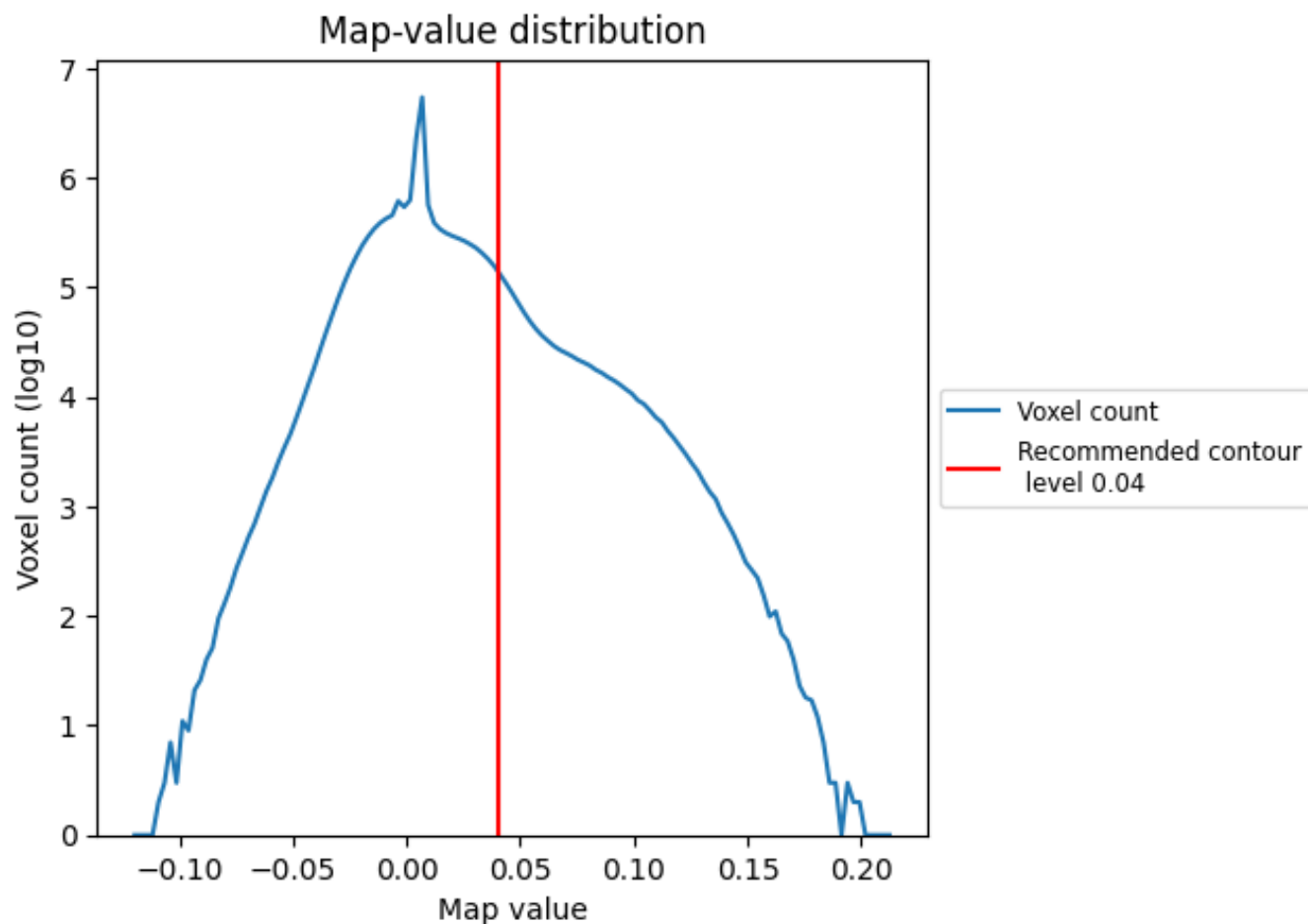
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

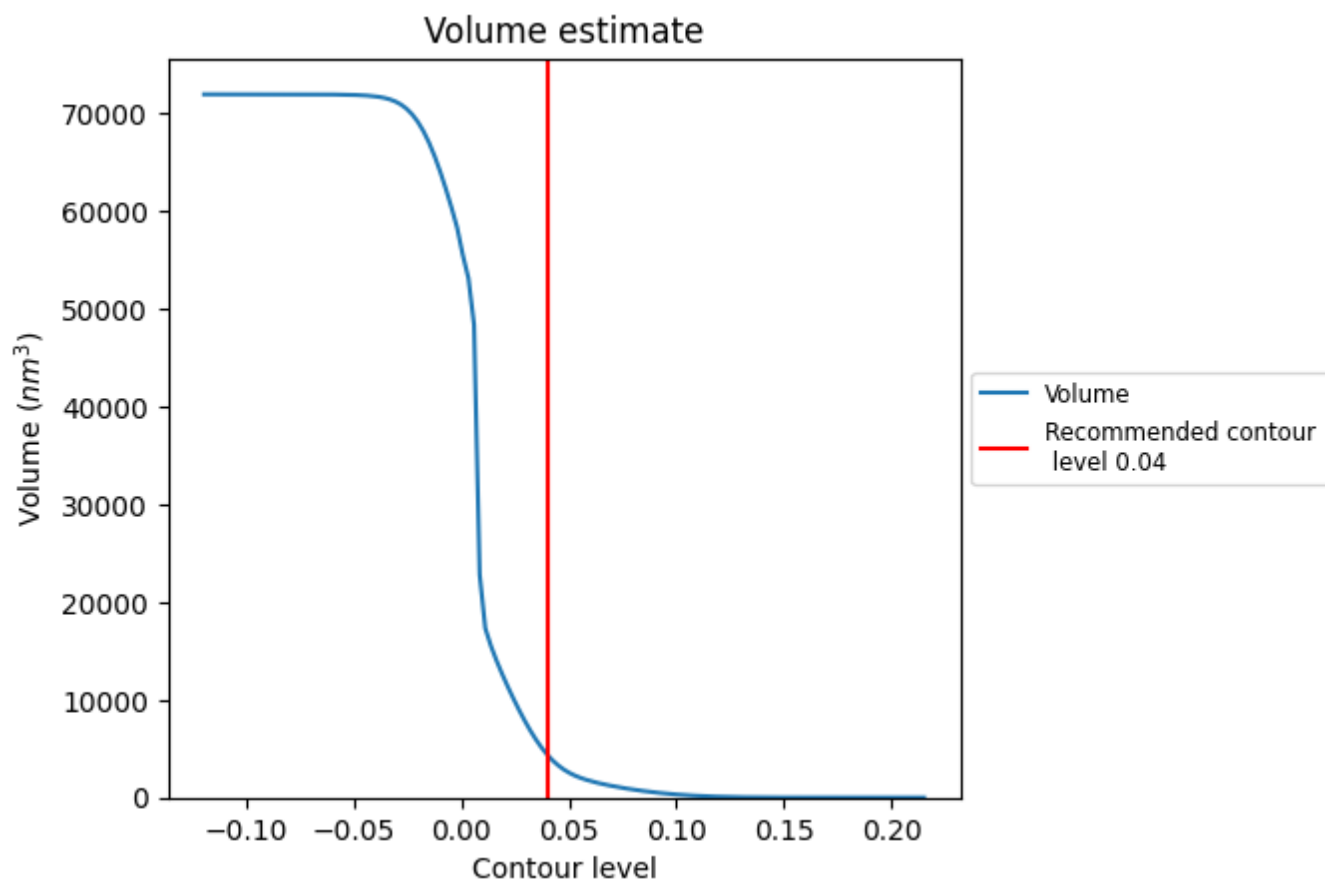
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

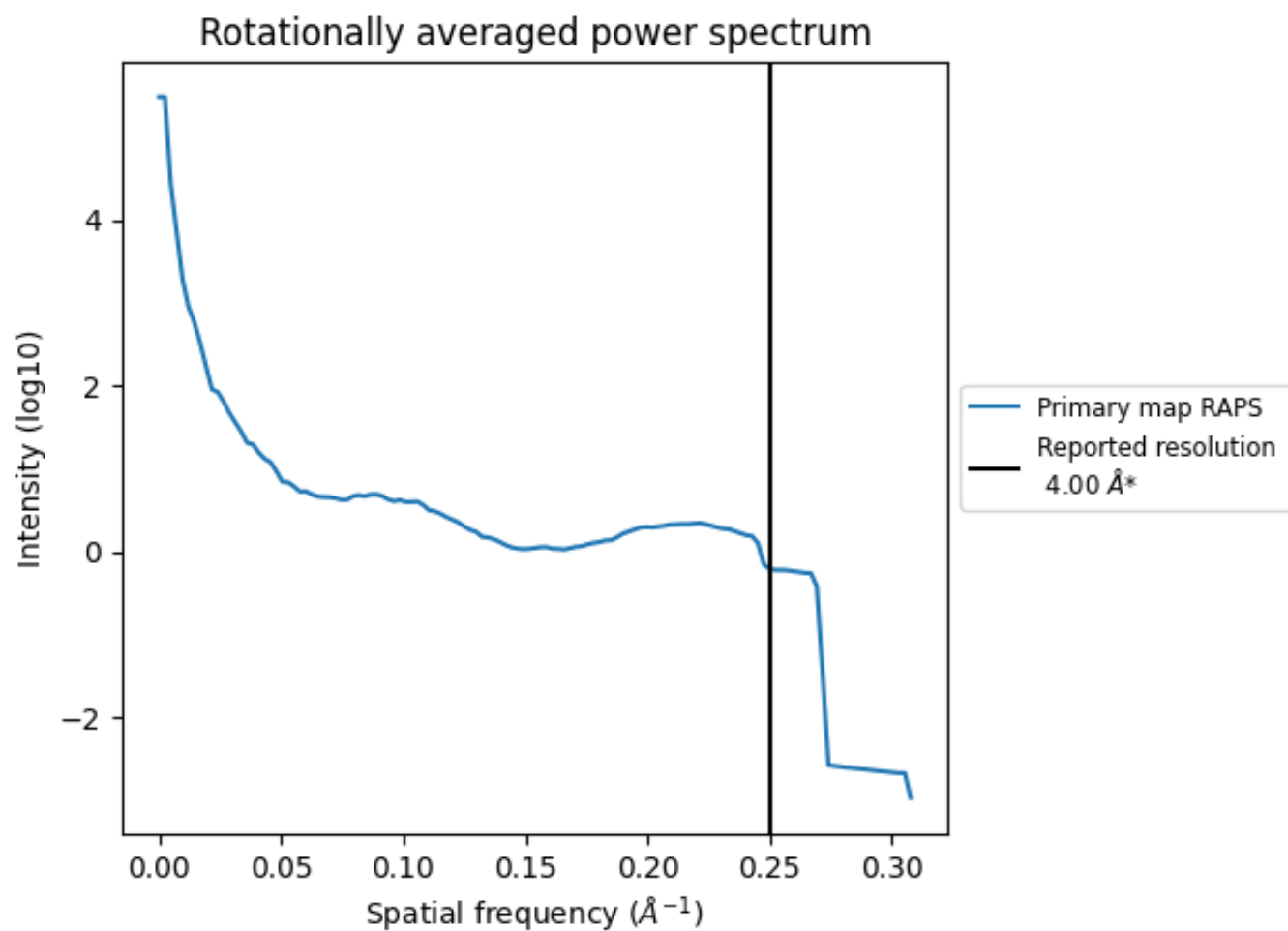
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4382 nm<sup>3</sup>; 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

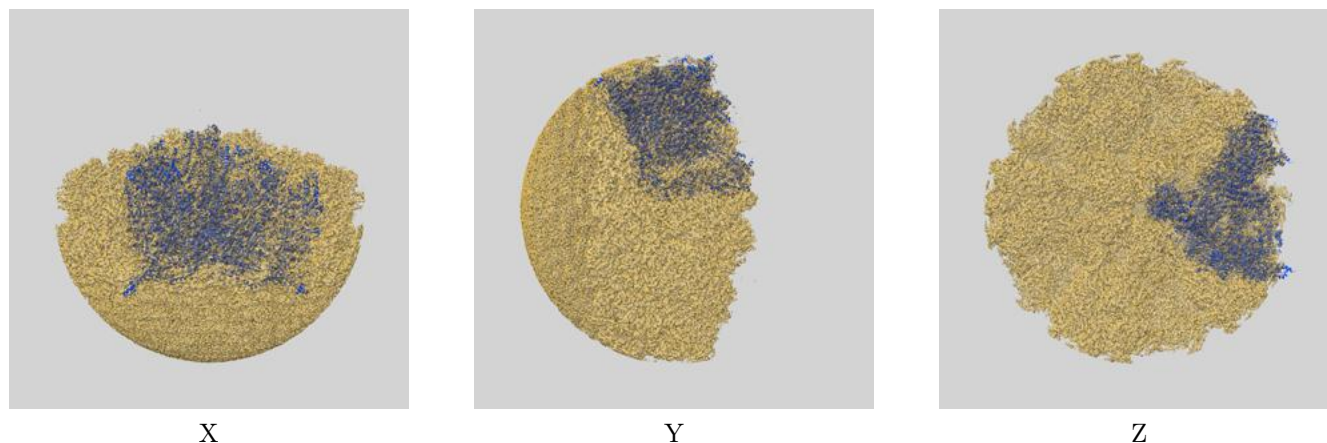
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

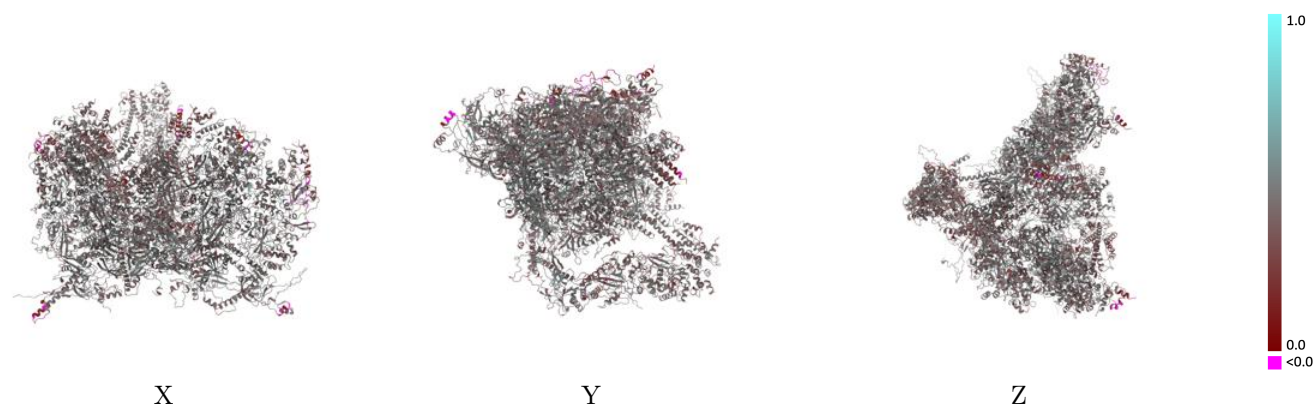
This section contains information regarding the fit between EMDB map EMD-31301 and PDB model 7ETO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



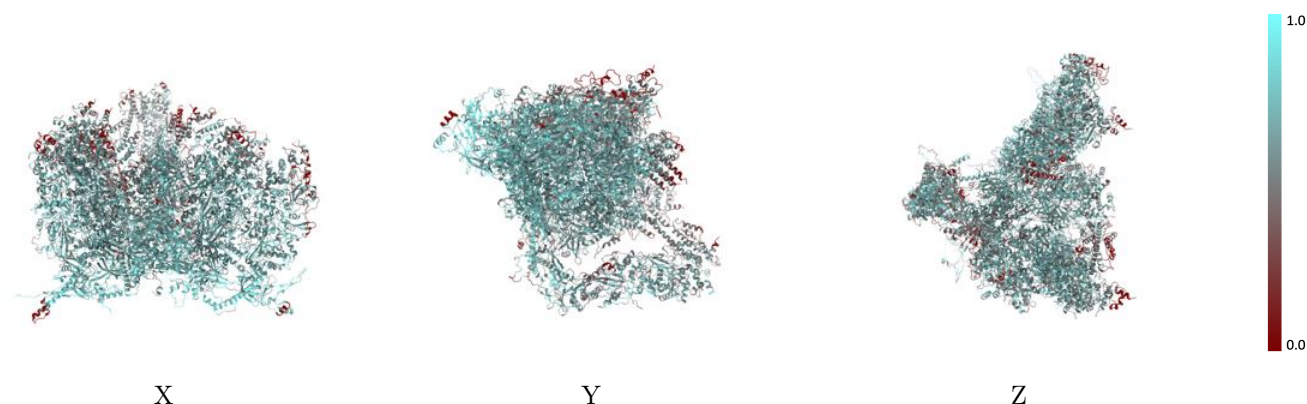
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



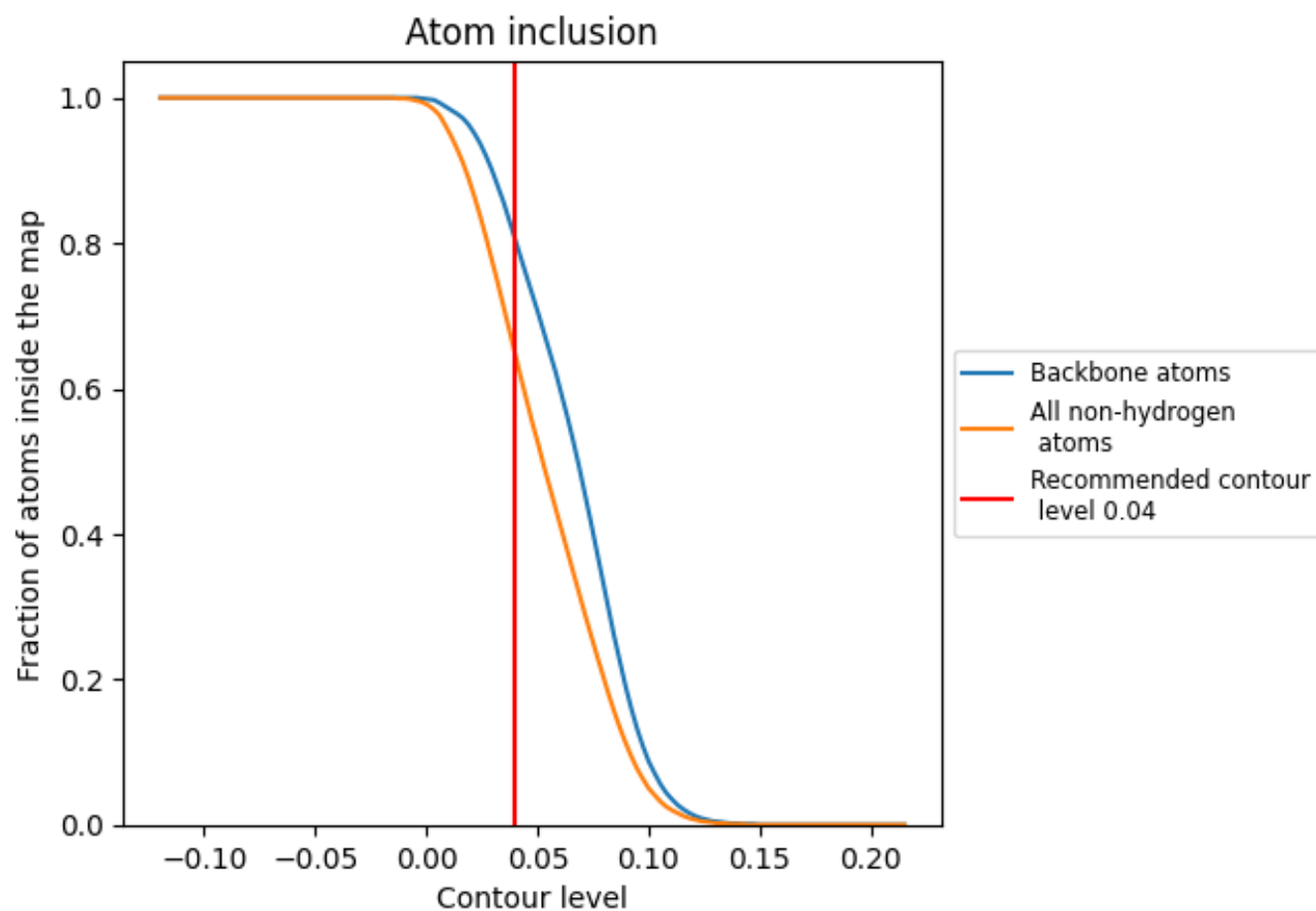
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 80% 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	 0.6470	 0.4280
1	 0.4150	 0.3720
A	 0.5930	 0.4080
B	 0.6670	 0.4410
C	 0.7080	 0.4480
D	 0.6840	 0.4390
H	 0.3530	 0.3050
I	 0.5970	 0.4120
M	 0.6780	 0.4310
N	 0.5460	 0.3660
O	 0.4110	 0.2970
P	 0.3890	 0.3220
Q	 0.4600	 0.3810
R	 0.4180	 0.3790
S	 0.4740	 0.3990
T	 0.2530	 0.2760
Y	 0.6620	 0.4200
Z	 0.6920	 0.4480
a	 0.7010	 0.4510
g	 0.6250	 0.4060
h	 0.6610	 0.4150
i	 0.3270	 0.3450
j	 0.4020	 0.3890
m	 0.7070	 0.4510
n	 0.6530	 0.4190
o	 0.6500	 0.4240
x	 0.4650	 0.3860

