



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 06:49 PM JST

PDB ID : 7ET3
EMDB ID : EMD-31297
Title : C5 portal vertex in the enveloped virion capsid
Authors : Li, Z.; Yu, X.
Deposited on : 2021-05-12
Resolution : 4.20 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

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:

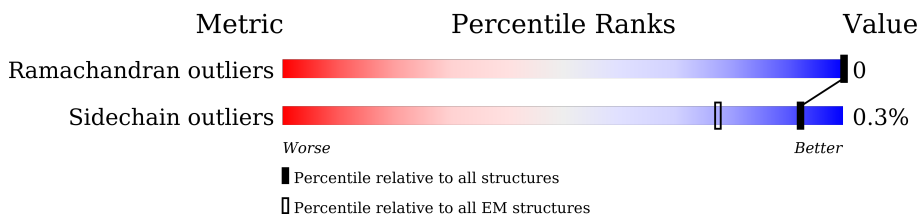
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 4.20 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	I	306	
1	h	306	
1	n	306	
1	o	306	
2	H	2241	
2	P	2241	
3	g	290	
3	m	290	
4	M	594	

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Mol	Chain	Length	Quality of chain
5	N	642	 10% 90%
5	O	642	 5% 11% 84%
6	1	1048	 8% 27% 65%
7	R	75	 31% 52% 17%
7	S	75	 17% 66% 17%
7	T	75	 57% 26% 17%
7	i	75	 40% 44% 16%
7	j	75	 25% 58% 17%
8	B	1370	 1% 96% 3%
8	C	1370	 1% 96% 3%
8	D	1370	 6% 88% 6%
8	Y	1370	 9% 89% 2%
8	Z	1370	 6% 91% 3%
8	a	1370	 1% 93% 6%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 86332 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 Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	h	285	Total 2258	C 1454	N 386	O 402	S 16	0	0
1	I	285	Total 2264	C 1454	N 389	O 404	S 17	0	0
1	n	293	Total 2322	C 1493	N 400	O 410	S 19	0	0
1	o	282	Total 2239	C 1442	N 382	O 397	S 18	0	0

- Molecule 2 is a protein called Large tegument protein deneddylase.

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

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	g	237	Total 1896	C 1218	N 332	O 335	S 11	0	0
3	m	290	Total 2325	C 1485	N 411	O 417	S 12	0	0

- Molecule 4 is a protein called Capsid vertex component 1.

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

- Molecule 5 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	65	Total	C	N	O	S	0	0
			551	341	110	96	4		
5	O	69	Total	C	N	O	S	0	0
			589	371	113	102	3		

- Molecule 6 is a protein called ORFL92C_UL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
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		

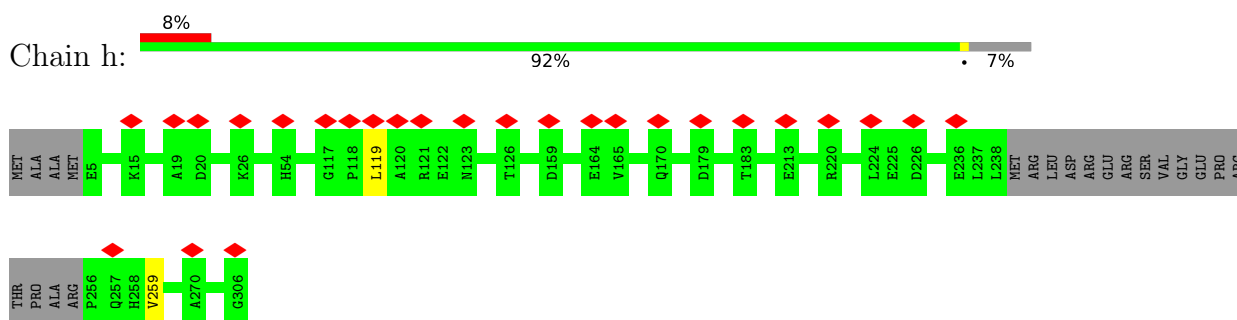
- Molecule 8 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	1286	Total	C	N	O	S	0	0
			10169	6469	1770	1871	59		
8	B	1332	Total	C	N	O	S	0	0
			10567	6728	1831	1947	61		
8	C	1330	Total	C	N	O	S	0	0
			10540	6713	1830	1936	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		
8	Z	1337	Total	C	N	O	S	0	0
			10582	6740	1831	1952	59		

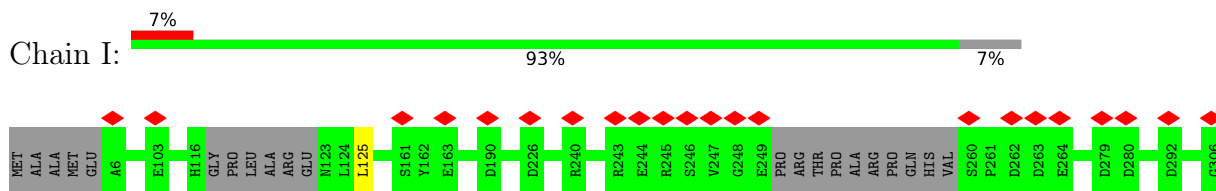
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

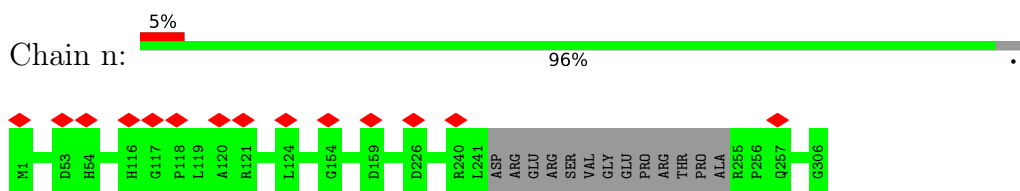
- Molecule 1: Triplex capsid protein 2



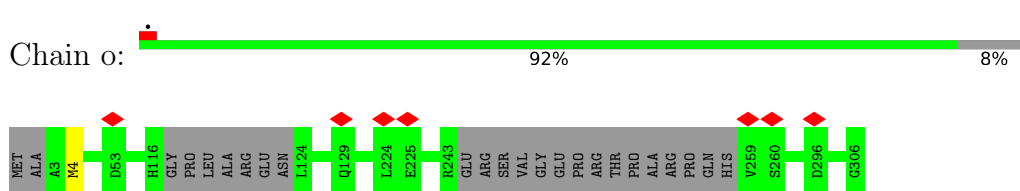
- Molecule 1: Triplex capsid protein 2



- Molecule 1: Triplex capsid protein 2

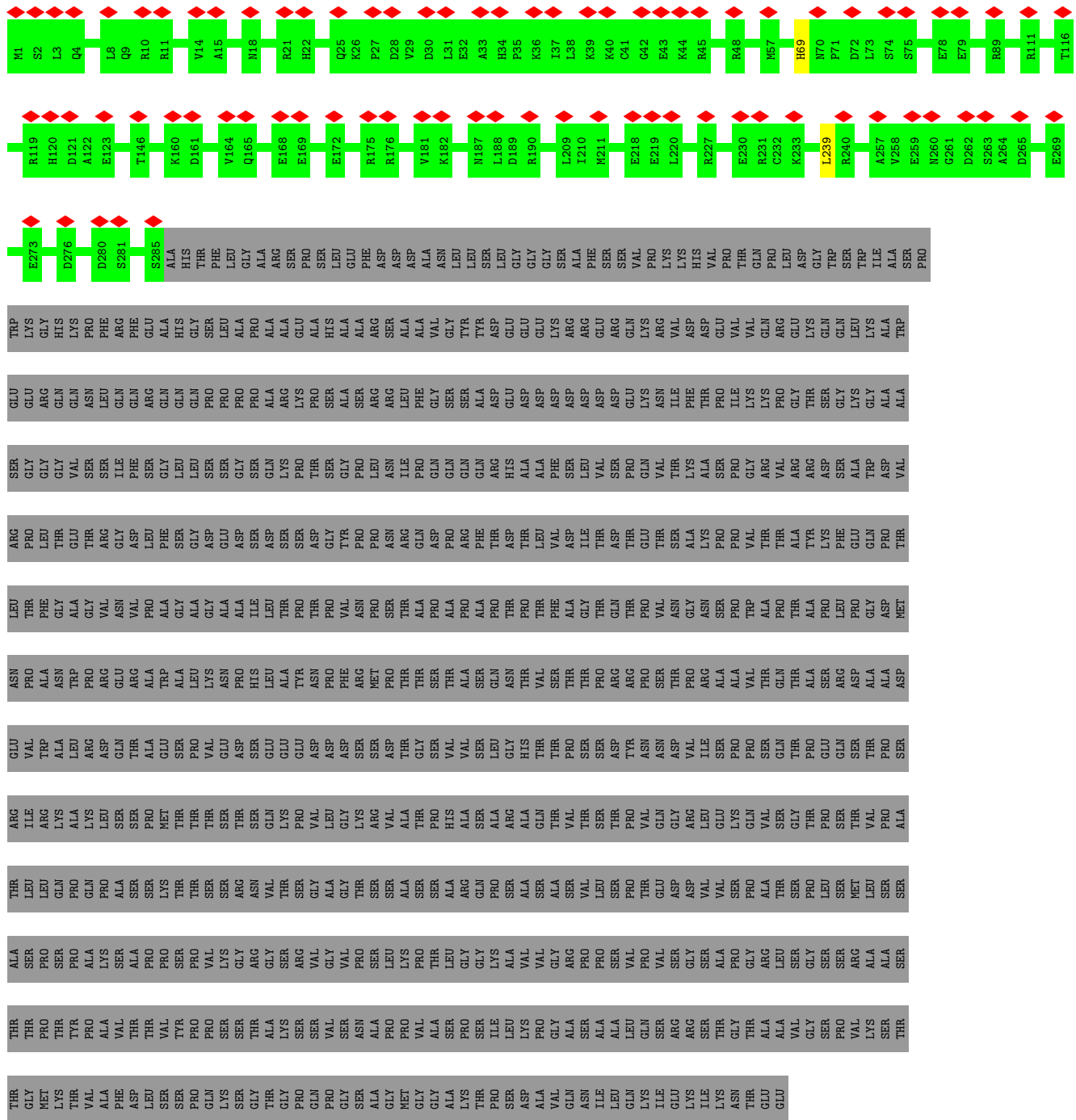


- Molecule 1: Triplex capsid protein 2

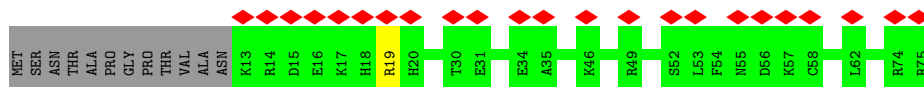
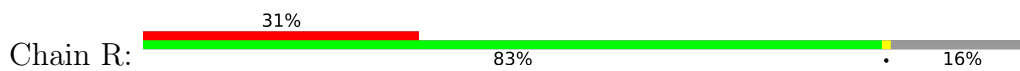


- Molecule 2: Large tegument protein deneddylase

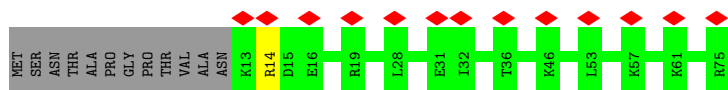
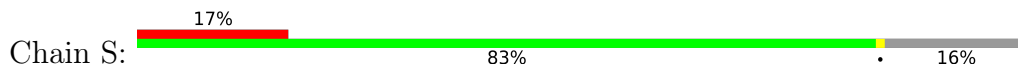




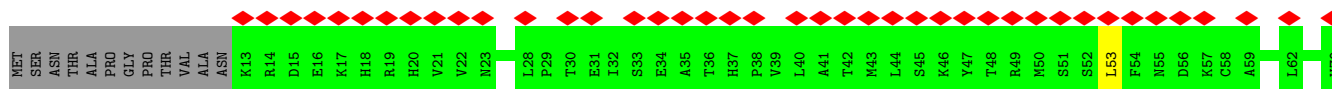
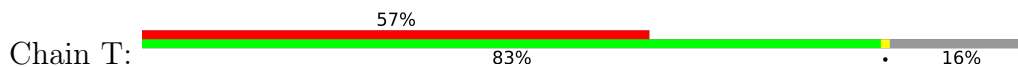
● Molecule 7: Small capsomere-interacting protein



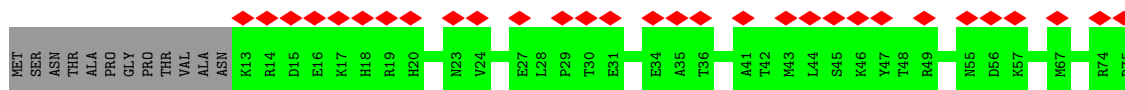
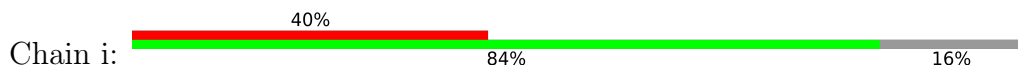
• Molecule 7: Small capsomere-interacting protein



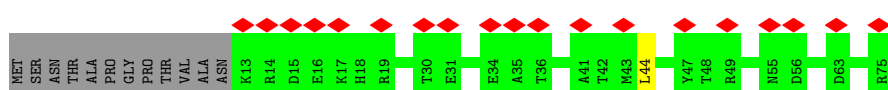
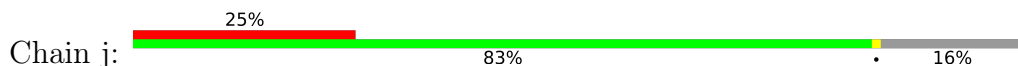
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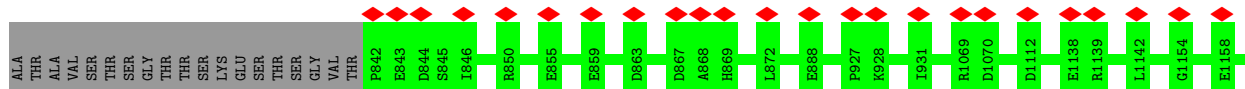
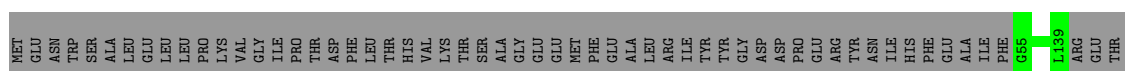
• Molecule 7: Small capsomere-interacting protein

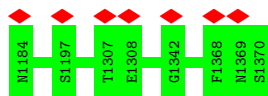


• Molecule 7: Small capsomere-interacting protein

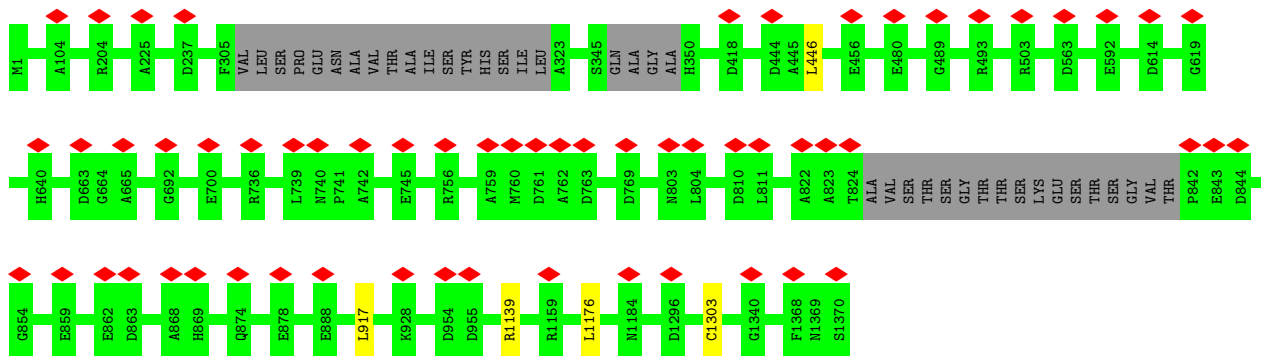


• Molecule 8: Major capsid protein

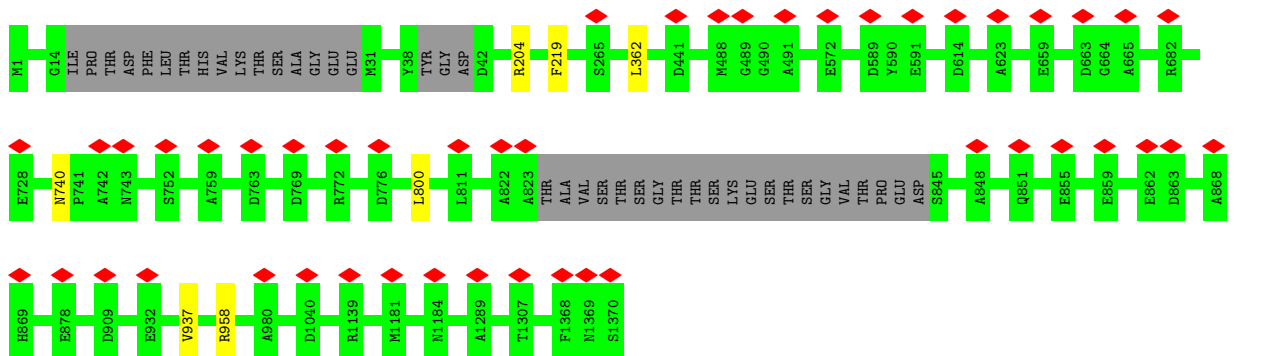




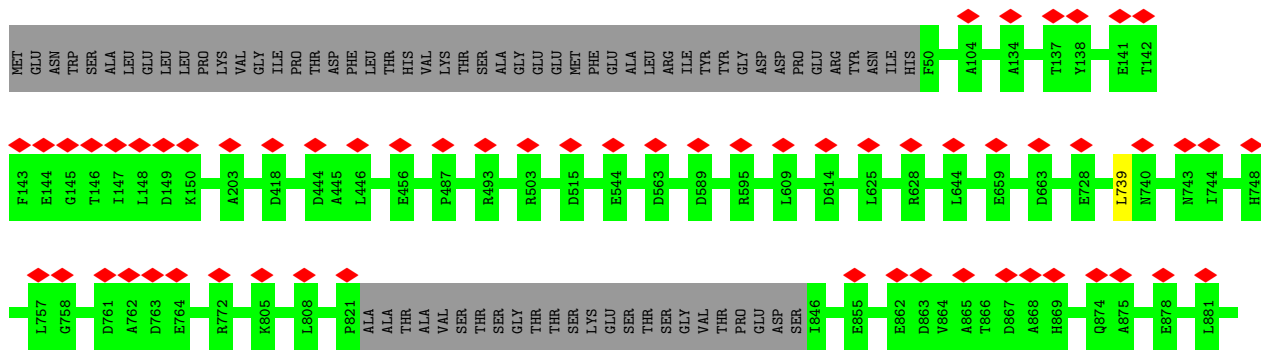
• Molecule 8: Major capsid protein

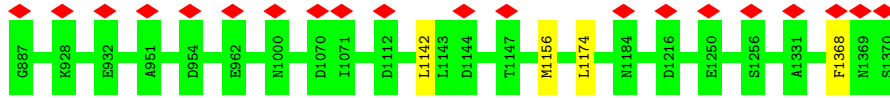


• Molecule 8: Major capsid protein

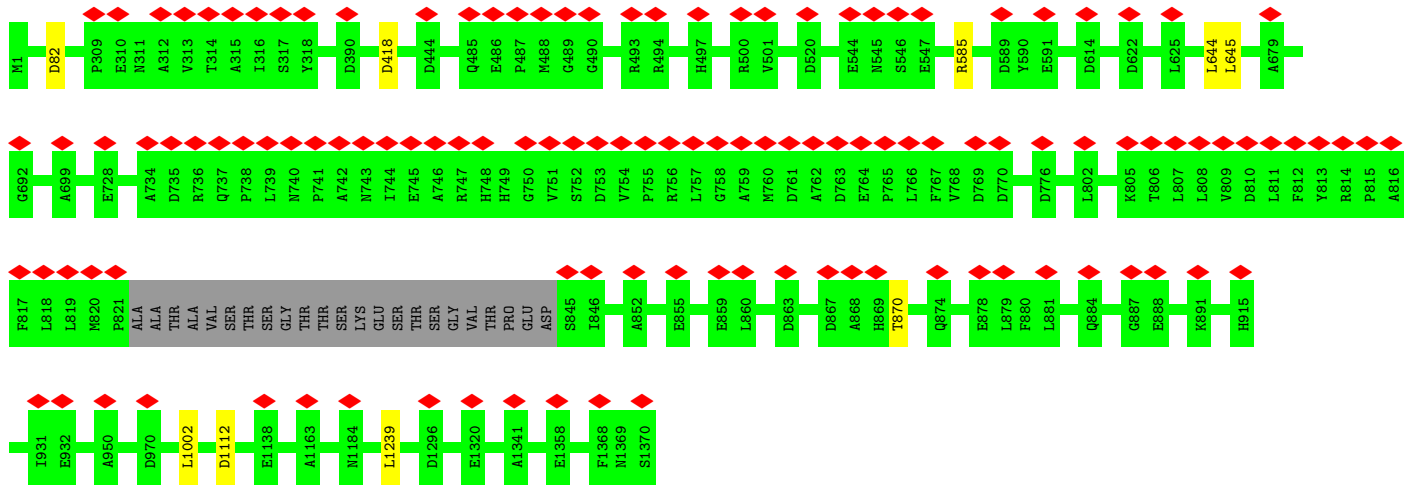


• Molecule 8: Major capsid protein

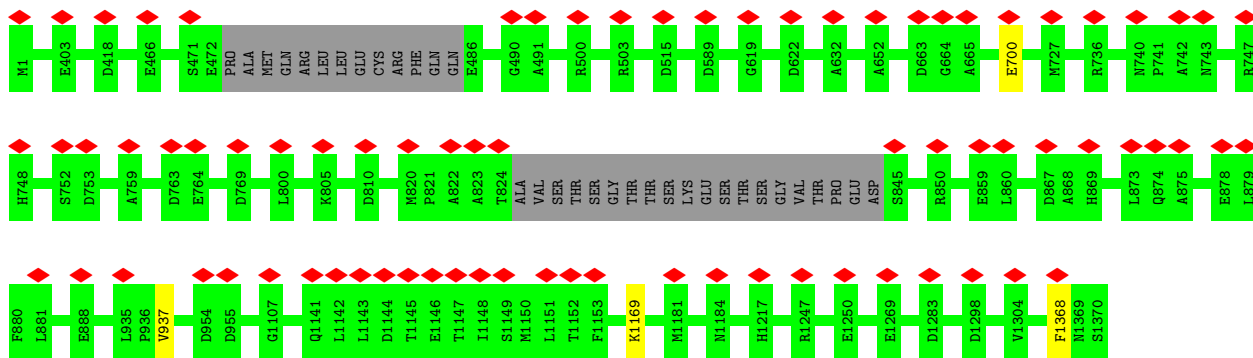




• Molecule 8: Major capsid protein



• 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	23136	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	0.075	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.01	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	I	0.29	0/2304	0.58	1/3125 (0.0%)
1	h	0.29	0/2302	0.60	1/3128 (0.0%)
1	n	0.29	0/2366	0.58	0/3212
1	o	0.30	0/2279	0.57	0/3092
2	H	0.29	0/174	0.56	0/233
2	P	0.28	0/174	0.50	0/233
3	g	0.29	0/1936	0.55	0/2625
3	m	0.30	0/2374	0.56	0/3221
4	M	0.30	0/3935	0.57	0/5331
5	N	0.31	0/560	0.60	0/751
5	O	0.29	0/600	0.62	1/808 (0.1%)
6	1	0.30	0/2366	0.59	1/3192 (0.0%)
7	R	0.26	0/520	0.58	0/697
7	S	0.28	0/520	0.56	0/697
7	T	0.28	0/520	0.61	1/697 (0.1%)
7	i	0.30	0/520	0.65	0/697
7	j	0.30	0/520	0.55	0/697
8	B	0.30	0/10819	0.55	3/14733 (0.0%)
8	C	0.30	0/10790	0.54	2/14695 (0.0%)
8	D	0.30	0/10513	0.56	3/14322 (0.0%)
8	Y	0.30	0/10932	0.55	2/14892 (0.0%)
8	Z	0.30	0/10835	0.55	1/14762 (0.0%)
8	a	0.31	0/10410	0.56	0/14183
All	All	0.30	0/88269	0.56	16/120023 (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
6	1	0	1
8	Y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	a	0	1
All	All	0	3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	h	119	LEU	CA-CB-CG	7.92	133.51	115.30
7	T	53	LEU	CA-CB-CG	6.74	130.80	115.30
8	D	1156	MET	CA-CB-CG	5.61	122.84	113.30
8	C	362	LEU	CA-CB-CG	5.48	127.91	115.30
8	Y	1002	LEU	CA-CB-CG	5.47	127.89	115.30
1	I	125	LEU	CA-CB-CG	5.41	127.73	115.30
8	B	917	LEU	CA-CB-CG	5.38	127.68	115.30
8	Y	645	LEU	CA-CB-CG	5.37	127.65	115.30
8	D	1174	LEU	CA-CB-CG	5.34	127.57	115.30
8	Z	700	GLU	C-N-CA	5.33	135.03	121.70
8	D	1142	LEU	CA-CB-CG	5.30	127.49	115.30
6	1	239	LEU	CA-CB-CG	5.24	127.36	115.30
8	C	800	LEU	CA-CB-CG	5.23	127.32	115.30
8	B	1176	LEU	CA-CB-CG	5.21	127.29	115.30
8	B	446	LEU	CA-CB-CG	5.10	127.04	115.30
5	O	68	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1	69	HIS	Peptide
8	Y	585	ARG	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

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	I	279/306 (91%)	264 (95%)	15 (5%)	0	100	100
1	h	281/306 (92%)	262 (93%)	19 (7%)	0	100	100
1	n	289/306 (94%)	267 (92%)	22 (8%)	0	100	100
1	o	276/306 (90%)	263 (95%)	13 (5%)	0	100	100
2	H	18/2241 (1%)	17 (94%)	1 (6%)	0	100	100
2	P	18/2241 (1%)	17 (94%)	1 (6%)	0	100	100
3	g	233/290 (80%)	214 (92%)	19 (8%)	0	100	100
3	m	288/290 (99%)	273 (95%)	15 (5%)	0	100	100
4	M	462/594 (78%)	432 (94%)	30 (6%)	0	100	100
5	N	63/642 (10%)	61 (97%)	2 (3%)	0	100	100
5	O	65/642 (10%)	64 (98%)	1 (2%)	0	100	100
6	l	283/1048 (27%)	270 (95%)	13 (5%)	0	100	100
7	R	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
7	S	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
7	T	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	i	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
7	j	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
8	B	1324/1370 (97%)	1245 (94%)	79 (6%)	0	100	100
8	C	1322/1370 (96%)	1244 (94%)	78 (6%)	0	100	100
8	D	1293/1370 (94%)	1228 (95%)	65 (5%)	0	100	100
8	Y	1343/1370 (98%)	1254 (93%)	89 (7%)	0	100	100
8	Z	1331/1370 (97%)	1252 (94%)	79 (6%)	0	100	100
8	a	1280/1370 (93%)	1192 (93%)	88 (7%)	0	100	100
All	All	10753/17807 (60%)	10113 (94%)	640 (6%)	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	I	257/273 (94%)	257 (100%)	0	100	100
1	h	256/273 (94%)	255 (100%)	1 (0%)	91	94
1	n	262/273 (96%)	262 (100%)	0	100	100
1	o	254/273 (93%)	253 (100%)	1 (0%)	91	94
2	H	19/1941 (1%)	19 (100%)	0	100	100
2	P	19/1941 (1%)	19 (100%)	0	100	100
3	g	207/252 (82%)	207 (100%)	0	100	100
3	m	252/252 (100%)	252 (100%)	0	100	100
4	M	395/500 (79%)	394 (100%)	1 (0%)	92	95
5	N	58/526 (11%)	58 (100%)	0	100	100
5	O	64/526 (12%)	64 (100%)	0	100	100
6	l	256/883 (29%)	256 (100%)	0	100	100
7	R	59/68 (87%)	58 (98%)	1 (2%)	60	78
7	S	59/68 (87%)	58 (98%)	1 (2%)	60	78
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	B	1162/1192 (98%)	1160 (100%)	2 (0%)	93	96
8	C	1158/1192 (97%)	1153 (100%)	5 (0%)	91	94
8	D	1130/1192 (95%)	1128 (100%)	2 (0%)	93	96
8	Y	1174/1192 (98%)	1168 (100%)	6 (0%)	88	93
8	Z	1163/1192 (98%)	1160 (100%)	3 (0%)	92	95
8	a	1120/1192 (94%)	1118 (100%)	2 (0%)	93	96
All	All	9501/15405 (62%)	9475 (100%)	26 (0%)	92	95

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	h	259	VAL
1	o	4	MET
4	M	53	ARG
7	R	19	ARG
7	S	14	ARG
7	j	44	LEU
8	a	477	ARG
8	a	493	ARG
8	B	1139	ARG
8	B	1303	CYS
8	C	204	ARG
8	C	219	PHE
8	C	740	ASN
8	C	937	VAL
8	C	958	ARG
8	D	739	LEU
8	D	1368	PHE
8	Y	82	ASP
8	Y	418	ASP
8	Y	644	LEU
8	Y	870	THR
8	Y	1112	ASP
8	Y	1239	LEU
8	Z	937	VAL
8	Z	1169	LYS
8	Z	1368	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	h	36	GLN
1	h	209	ASN
1	I	285	GLN
2	H	2229	GLN
1	n	43	HIS
1	n	50	GLN
1	n	79	ASN
1	n	277	GLN
1	n	297	ASN
1	o	7	ASN
1	o	147	ASN

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Mol	Chain	Res	Type
1	o	235	GLN
1	o	297	ASN
3	g	211	HIS
3	g	232	ASN
3	m	240	GLN
3	m	249	GLN
4	M	322	HIS
4	M	571	HIS
6	1	170	ASN
6	1	177	ASN
6	1	201	ASN
7	R	37	HIS
7	T	55	ASN
7	i	23	ASN
8	a	81	HIS
8	a	208	ASN
8	a	217	GLN
8	a	341	ASN
8	a	438	GLN
8	a	534	HIS
8	a	541	HIS
8	a	545	ASN
8	a	620	ASN
8	a	694	ASN
8	a	849	GLN
8	a	869	HIS
8	a	919	ASN
8	a	940	HIS
8	a	945	ASN
8	a	1000	ASN
8	a	1003	HIS
8	a	1061	ASN
8	a	1275	ASN
8	B	208	ASN
8	B	257	ASN
8	B	534	HIS
8	B	618	HIS
8	B	749	HIS
8	B	1027	HIS
8	B	1100	ASN
8	B	1124	HIS
8	B	1264	GLN

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Mol	Chain	Res	Type
8	B	1309	GLN
8	B	1319	GLN
8	B	1350	HIS
8	C	194	GLN
8	C	208	ASN
8	C	338	HIS
8	C	346	GLN
8	C	510	ASN
8	C	514	GLN
8	C	618	HIS
8	C	673	HIS
8	C	708	ASN
8	C	903	GLN
8	C	919	ASN
8	C	940	HIS
8	C	1093	ASN
8	C	1111	GLN
8	C	1166	HIS
8	C	1190	ASN
8	C	1223	GLN
8	C	1309	GLN
8	C	1363	GLN
8	C	1364	GLN
8	D	76	HIS
8	D	81	HIS
8	D	205	GLN
8	D	257	ASN
8	D	341	ASN
8	D	346	GLN
8	D	534	HIS
8	D	543	GLN
8	D	560	ASN
8	D	637	ASN
8	D	660	HIS
8	D	737	GLN
8	D	794	ASN
8	D	945	ASN
8	D	1000	ASN
8	D	1093	ASN
8	D	1111	GLN
8	D	1229	HIS
8	D	1235	GLN

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Mol	Chain	Res	Type
8	D	1350	HIS
8	Y	3	ASN
8	Y	153	ASN
8	Y	194	GLN
8	Y	199	ASN
8	Y	422	ASN
8	Y	476	GLN
8	Y	484	GLN
8	Y	534	HIS
8	Y	637	ASN
8	Y	889	HIS
8	Y	914	GLN
8	Y	940	HIS
8	Y	1003	HIS
8	Y	1230	ASN
8	Y	1313	ASN
8	Y	1319	GLN
8	Y	1350	HIS
8	Z	47	ASN
8	Z	76	HIS
8	Z	214	ASN
8	Z	217	GLN
8	Z	257	ASN
8	Z	497	HIS
8	Z	534	HIS
8	Z	676	ASN
8	Z	849	GLN
8	Z	919	ASN
8	Z	969	HIS
8	Z	1029	HIS
8	Z	1093	ASN
8	Z	1223	GLN
8	Z	1248	HIS
8	Z	1350	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.

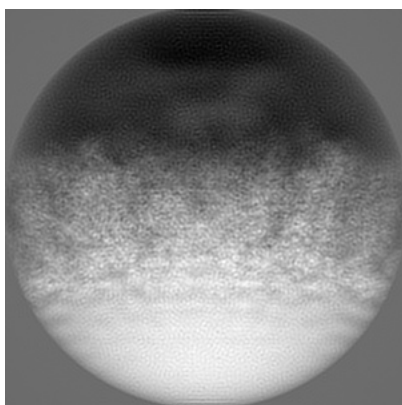
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31297. These allow visual inspection of the internal detail of the map and identification of artifacts.

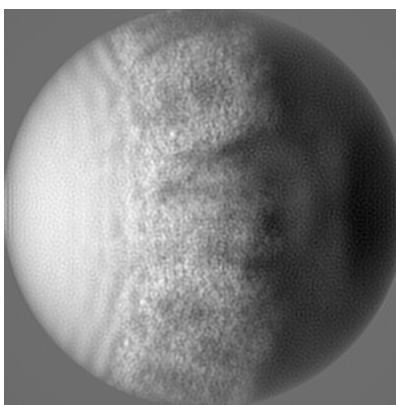
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

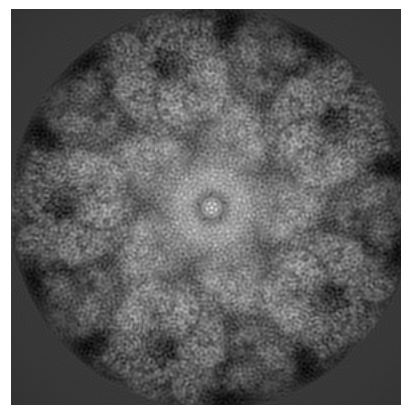
6.1.1 Primary map



X



Y

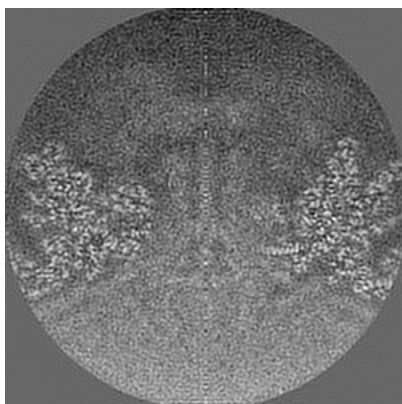


Z

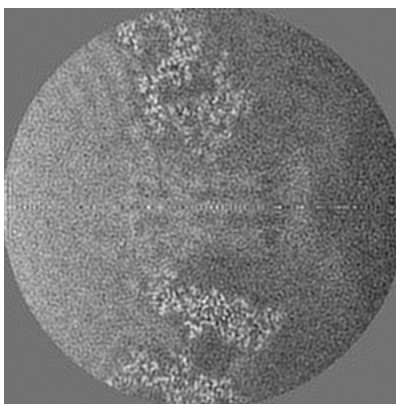
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

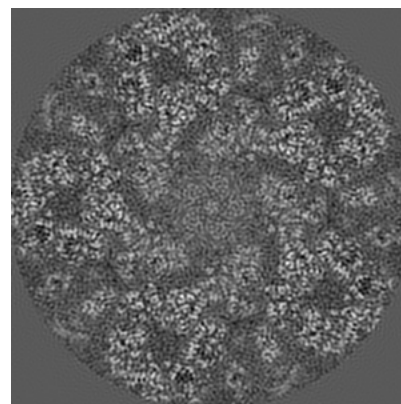
6.2.1 Primary map



X Index: 128



Y Index: 128

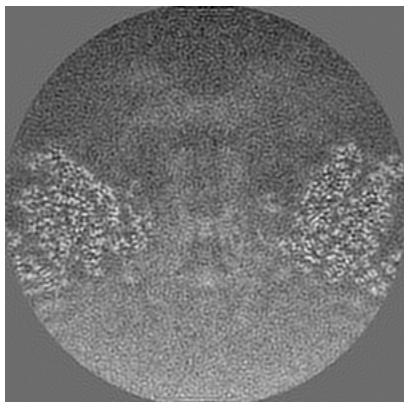


Z Index: 128

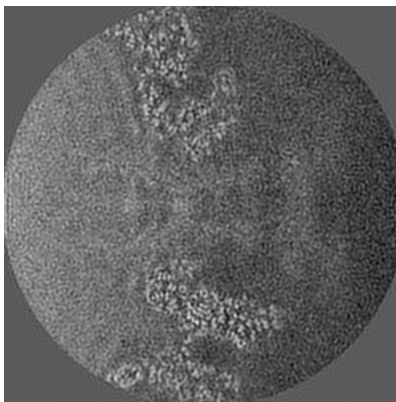
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

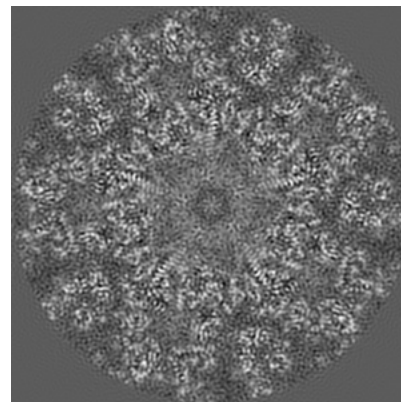
6.3.1 Primary map



X Index: 123



Y Index: 123

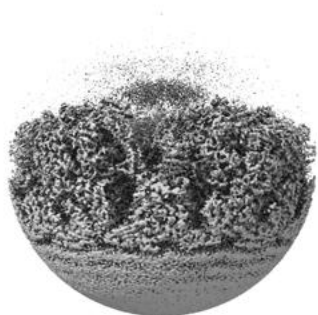


Z Index: 101

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

6.4 Orthogonal surface views [i](#)

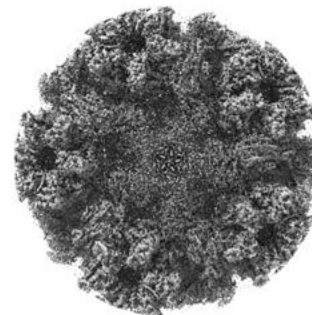
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

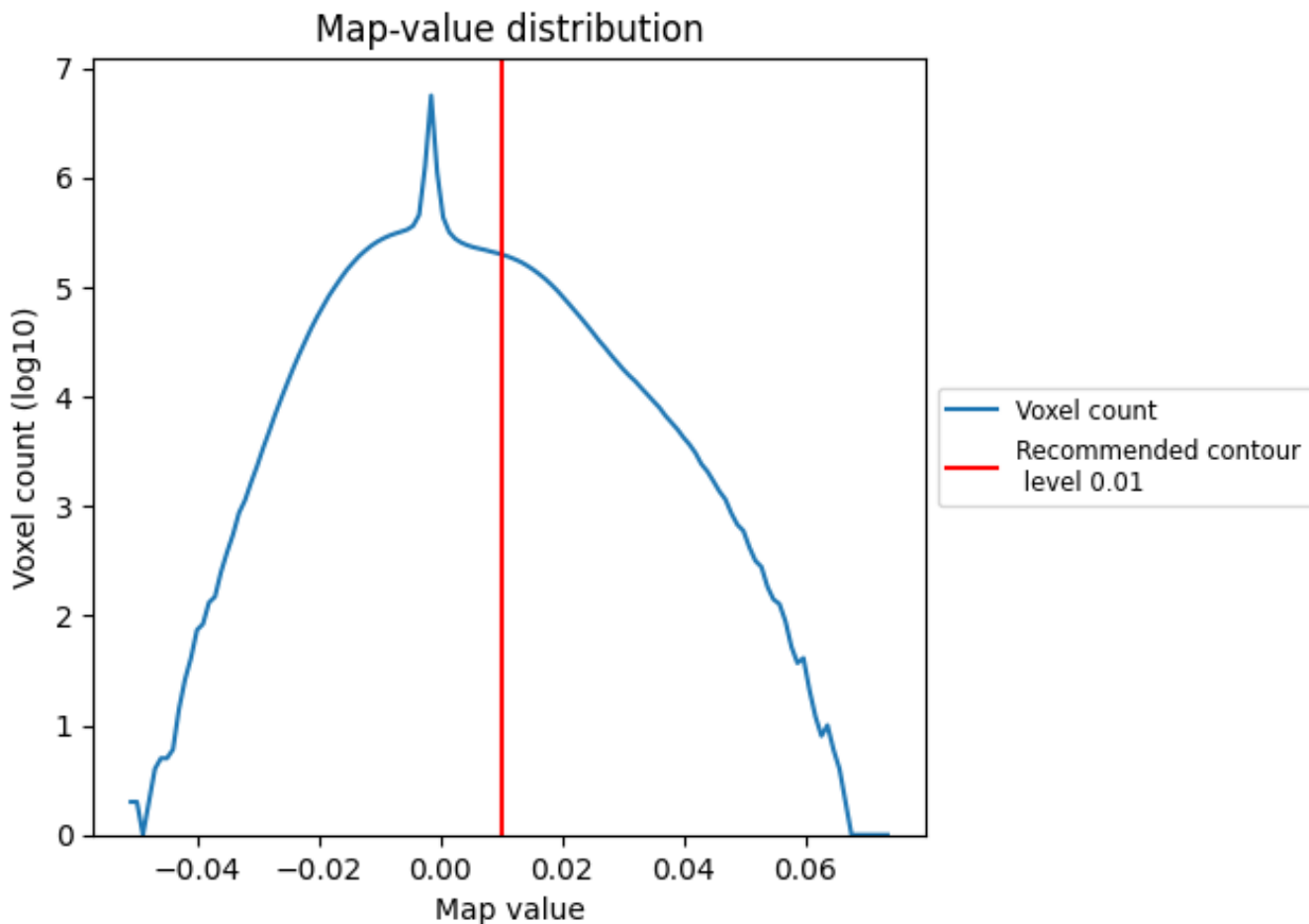
6.5 Mask visualisation

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

7 Map analysis [i](#)

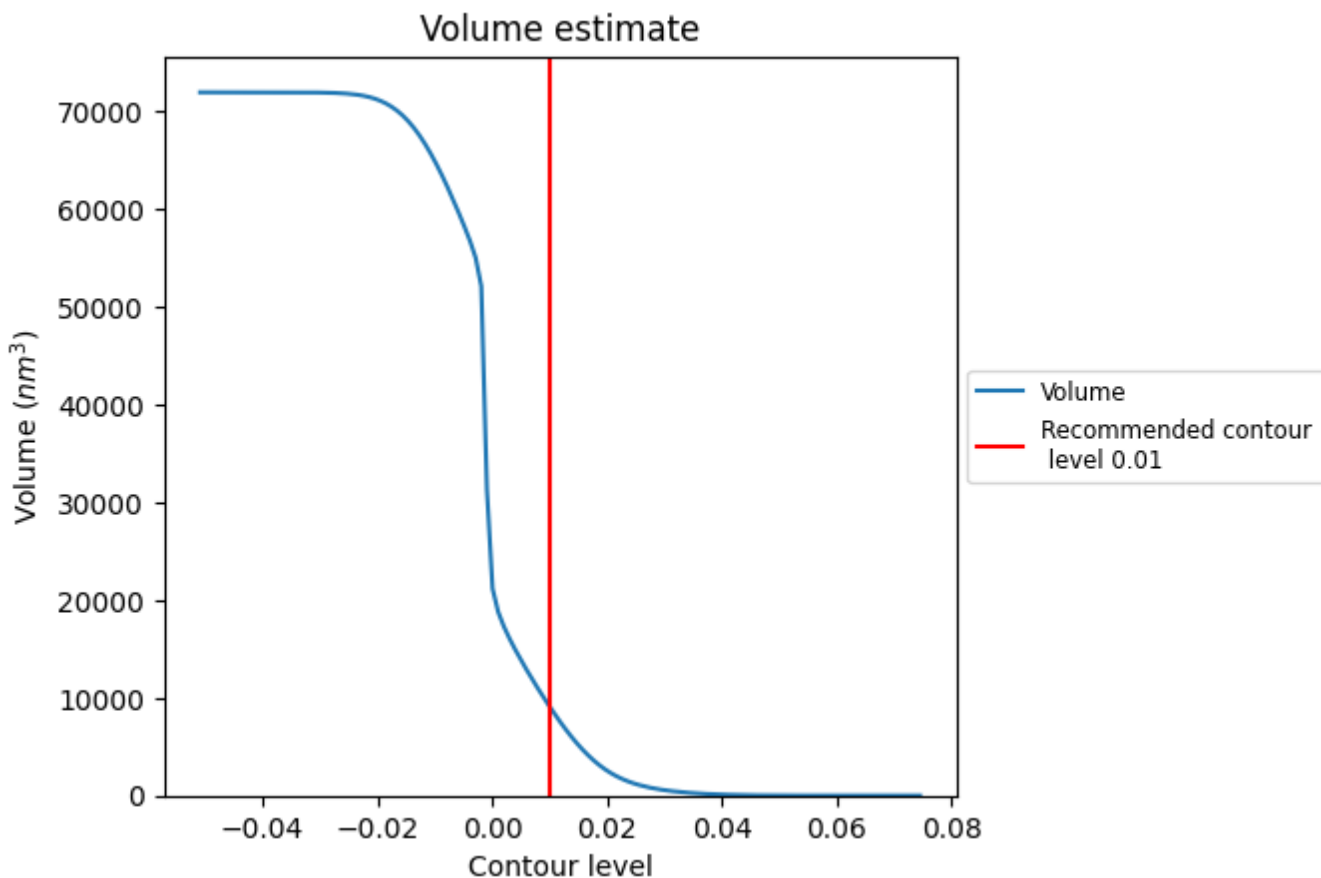
This section contains the results of statistical analysis of the map.

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.

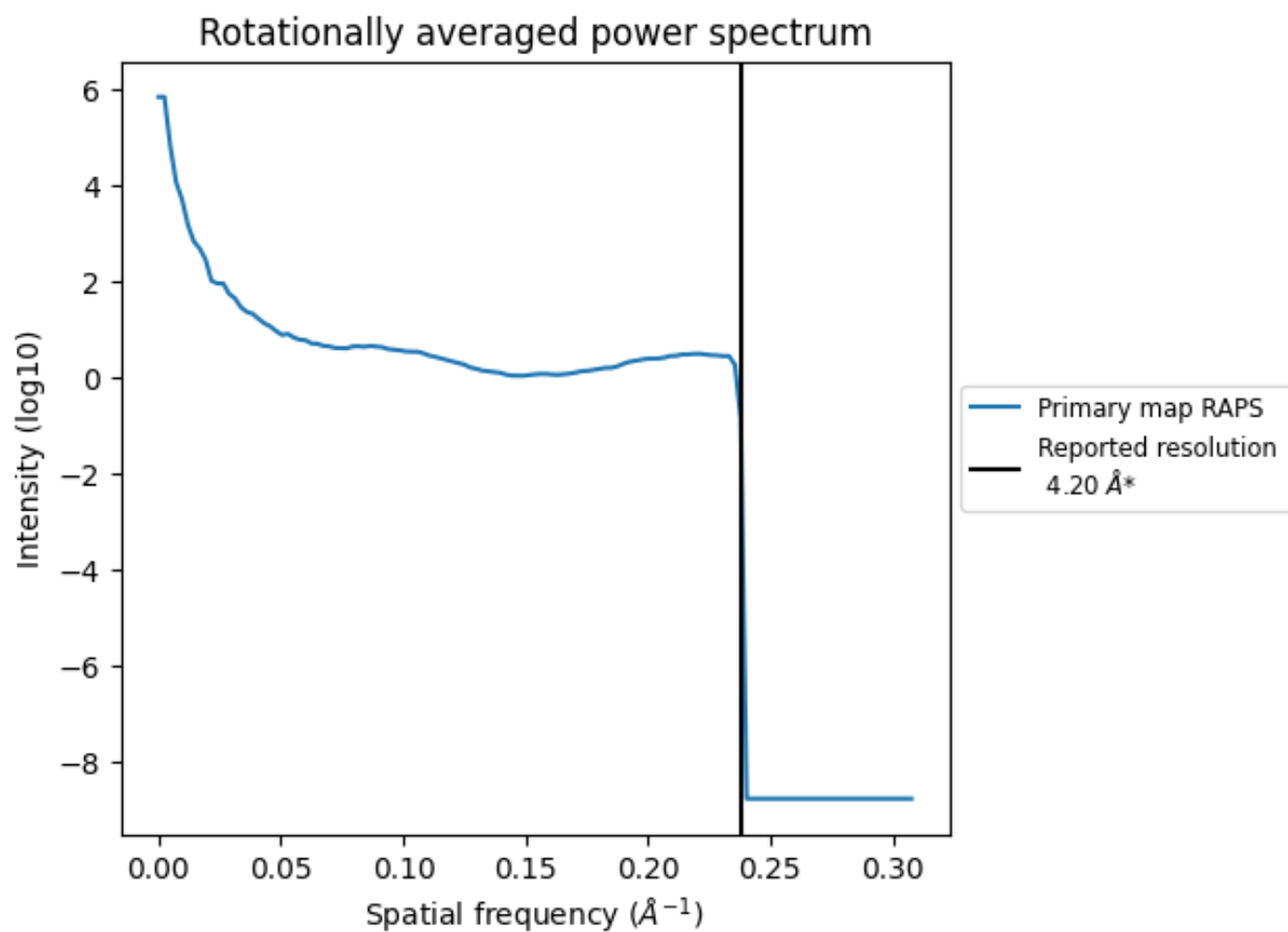
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9110 nm³; this corresponds to an approximate mass of 8230 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 0.238 Å⁻¹

8 Fourier-Shell correlation

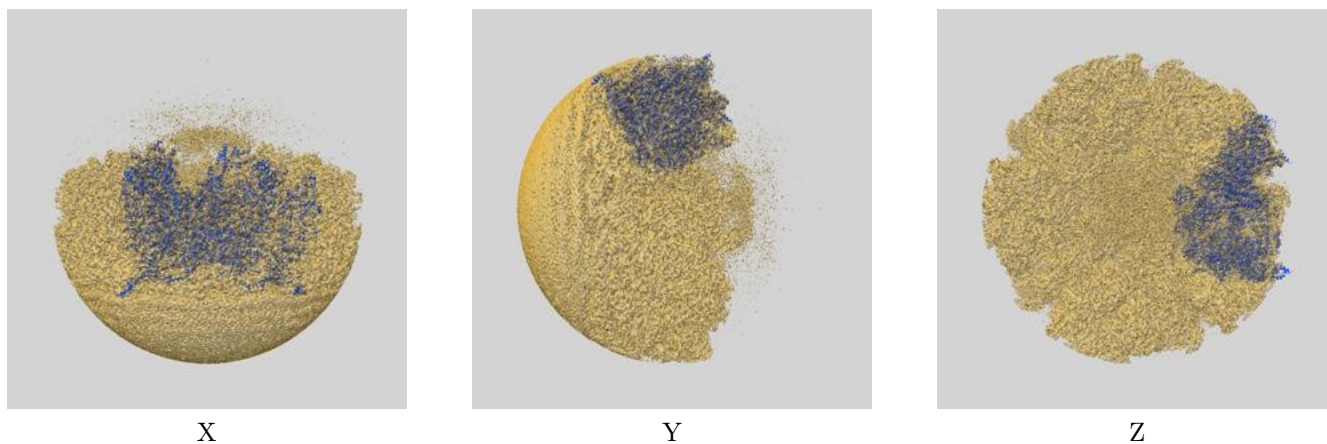
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

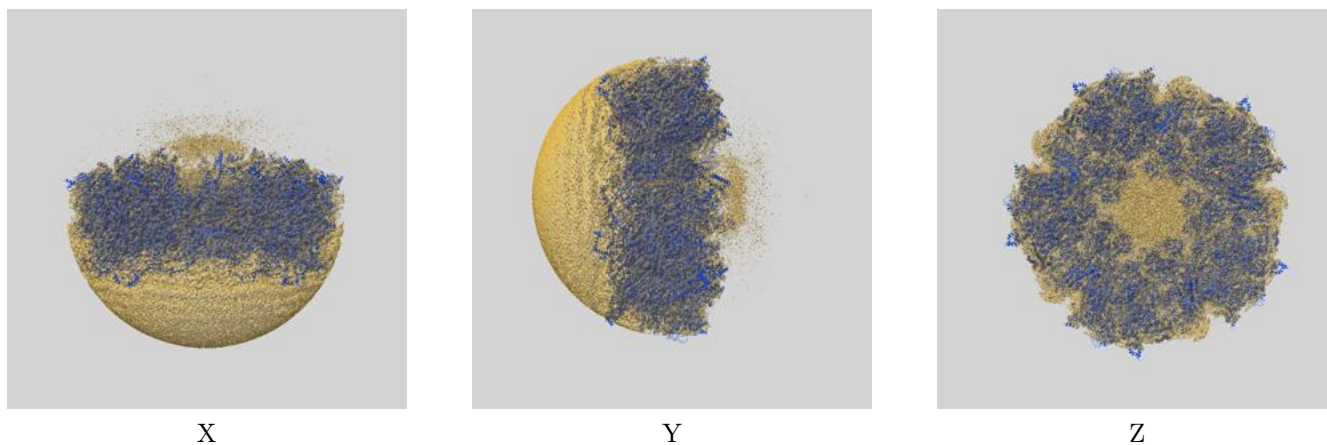
This section contains information regarding the fit between EMDB map EMD-31297 and PDB model 7ET3. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

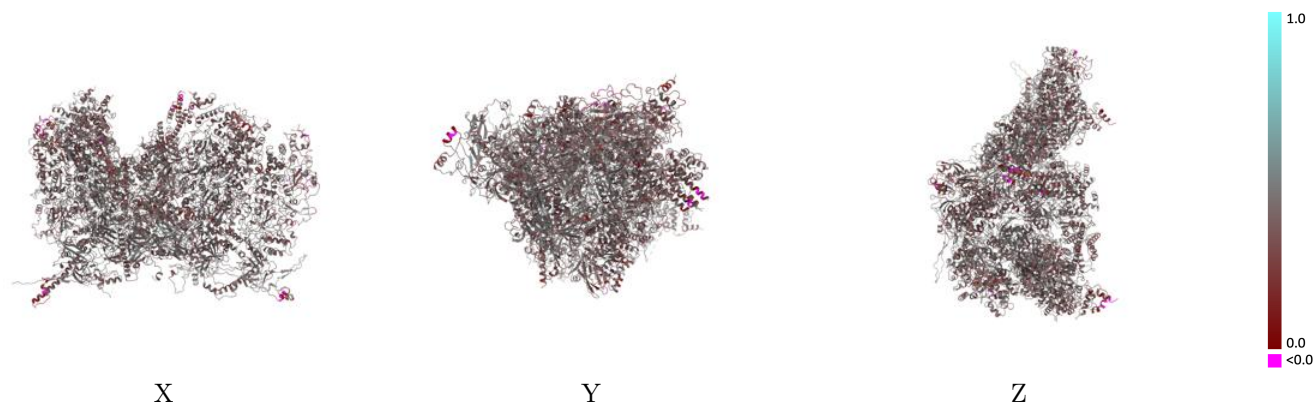


9.1.2 Map-model assembly overlay [i](#)



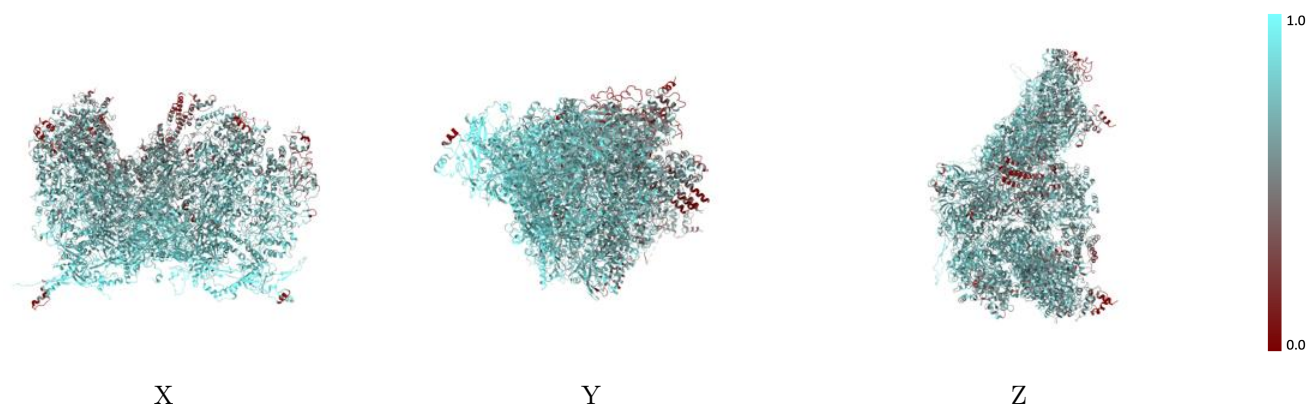
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



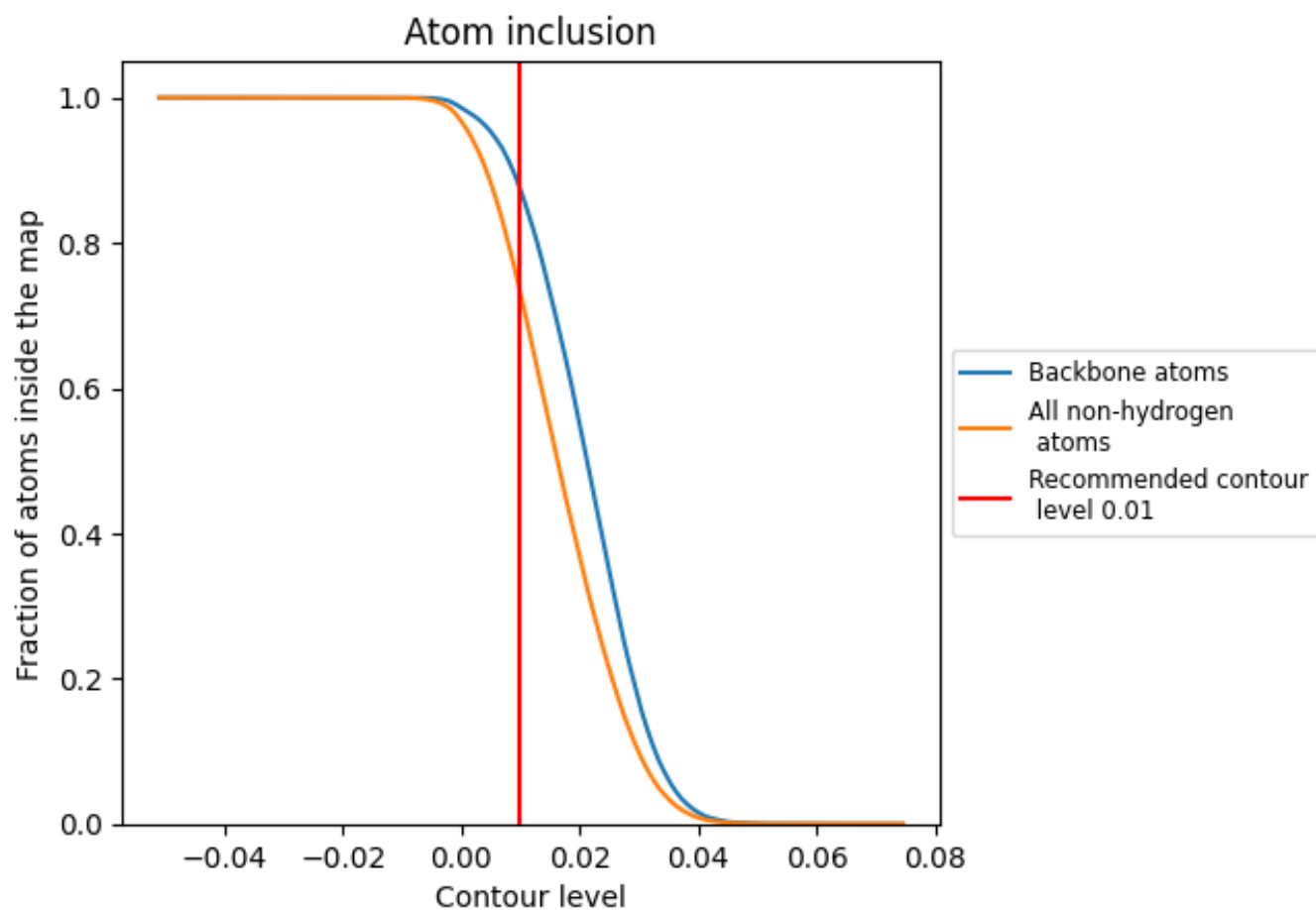
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 73% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.3980
1	 0.5498	 0.3720
B	 0.7678	 0.4060
C	 0.7791	 0.4130
D	 0.7546	 0.4000
H	 0.2874	 0.3060
I	 0.7255	 0.3830
M	 0.6010	 0.3910
N	 0.4523	 0.3440
O	 0.3989	 0.3210
P	 0.2635	 0.2900
R	 0.4779	 0.3630
S	 0.5201	 0.3800
T	 0.2791	 0.2660
Y	 0.7390	 0.3930
Z	 0.7650	 0.4070
a	 0.7751	 0.4090
g	 0.6772	 0.3630
h	 0.7023	 0.3750
i	 0.3594	 0.3420
j	 0.4900	 0.3610
m	 0.8032	 0.4100
n	 0.7570	 0.4000
o	 0.7735	 0.4000

