

Full wwPDB EM Validation Report (i)

Nov 22, 2022 – 06:58 PM JST

PDB ID : 7ETJ

EMDB ID : EMD-31298

Title: C5 portal vertex in the partially-enveloped virion capsid

 $\begin{array}{cccc} \text{Authors} & : & \text{Li, Z.; Yu, X.} \\ \text{Deposited on} & : & 2021\text{-}05\text{-}13 \end{array}$

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*A user guide is available at

https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) 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)

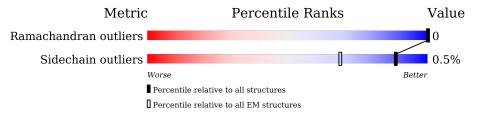
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance (i)

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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
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 <=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	98%	
1	h	306	98%	
1	n	306	95%	
1	О	306	94%	6%
2	Н	2241	• 99%	
2	Р	2241	99%	
3	g	290	78%	22%
3	m	290	99%	
4	M	594	6% 78%	21%

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Mol	Chain	Length	Quality of chain	
5	N	642	12% 88%	
5	О	642	11% 89%	
6	1	1048	10% 27% 73%	
7	R	75	27%	16%
7	S	75	84%	16%
7	Т	75	81% •	16%
7	i	75	81% ·	16%
7	j	75	35% 83%	16%
8	В	1370	97%	
8	С	1370	96%	
8	D	1370	94%	• 5%
8	Y	1370	98%	
8	Z	1370	97%	
8	a	1370	92%	• 7%



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 86613 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		At	oms			AltConf	Trace
1	h	300	Total	С	N	О	S	0	0
1	11	300	2384	1528	415	424	17	0	0
1	Т	301	Total	С	N	О	S	0	0
1	1	301	2389	1531	417	424	17	0	0
1	n	294	Total	С	N	О	S	0	0
1	n	294	2329	1499	401	410	19	0	0
1	0	289	Total	С	N	О	S	0	0
1	О	209	2291	1473	393	407	18	0	0

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

Mol	Chain	Residues		Ato	ms	AltConf	Trace		
2	Н	20	Total 172	_		_	S 1	0	0
2	Р	20	Total 172	_		_	S 1	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
2	ď	227	Total	С	N	О	S	0	0
)	3 g	221	1822	1171	319	321	11	0	
2	m	290	Total	С	N	О	S	0	0
)	m	290	2325	1485	411	417	12	0	0

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

Mol	Chain	Residues		At	AltConf	Trace			
4	М	468	Total	С	N	О	S	0	0
4	101	400	3848	2408	740	686	14	U	U

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



Mo	l Chain	Residues		At	oms	AltConf	Trace		
5	N	76	Total	С	N	О	S	0	0
)	9 1	10	648	408	127	109	4	0	
5	0	69	Total	С	N	О	S	0	0
)		09	589	371	113	102	3	0	0

 \bullet Molecule 6 is a protein called ORFL92C_UL32.

Mol	Chain	Residues		At	AltConf	Trace			
6	1	284	Total 2320	C 1463	N 425	O 420	S 12	0	0

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

Mol	Chain	Residues		Ato	ms		AltConf	Trace	
7	R	63	Total	С	N	О	S	0	0
'	n	0.0	513	321	97	91	4	0	0
7	S	63	Total	С	N	О	S	0	0
'	B	0.5	513	321	97	91	4	0	U
7	Т	63	Total	С	N	О	S	0	0
'	1	0.5	513	321	97	91	4	0	0
7	i	63	Total	С	N	О	S	0	0
'	1	0.5	513	321	97	91	4	0	U
7	;	63	Total	С	N	О	S	0	0
	J	00	513	321	97	91	4	U	U

• Molecule 8 is a protein called Major capsid protein.

Mol	Chain	Residues		A	$\overline{ ext{toms}}$			AltConf	Trace
8	a	1275	Total	С	N	О	S	0	0
0	a	1275	10079	6410	1756	1855	58		
8	В	1339	Total	С	N	О	S	0	0
6	Б	1559	10617	6762	1838	1956	61	U	U
8	С	1331	Total	С	N	O	S	0	0
0		1991	10536	6711	1827	1938	60		
8	D	1297	Total	С	N	О	S	0	0
	D	1291	10269	6538	1785	1887	59	0	U
8	Y	1347	Total	С	N	O	S	0	0
	1	1941	10676	6799	1850	1966	61	0	U
8	Z	1337	Total	С	N	О	S	0	0
		1001	10582	6740	1831	1952	59	0	U

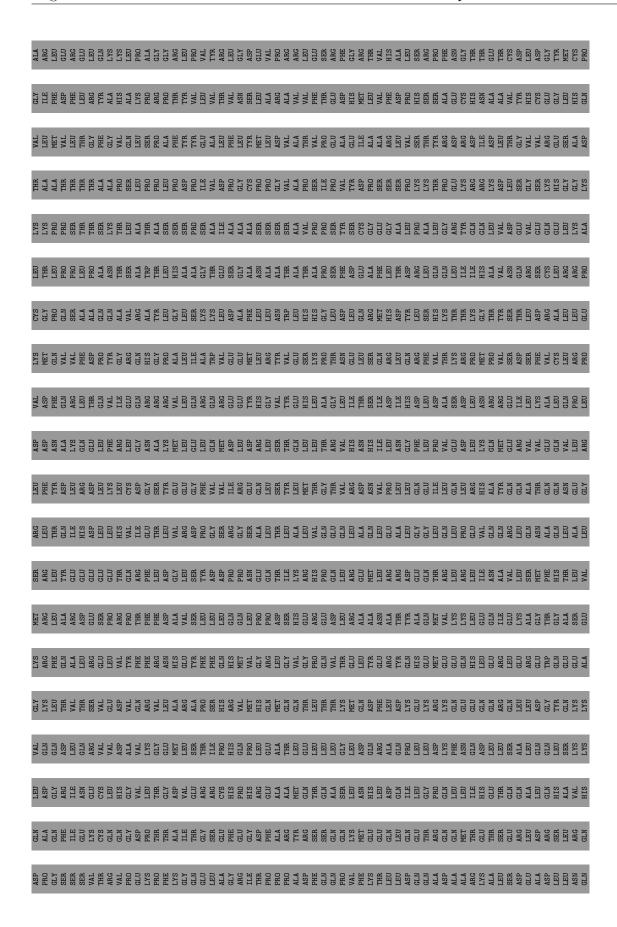


3 Residue-property plots (i)

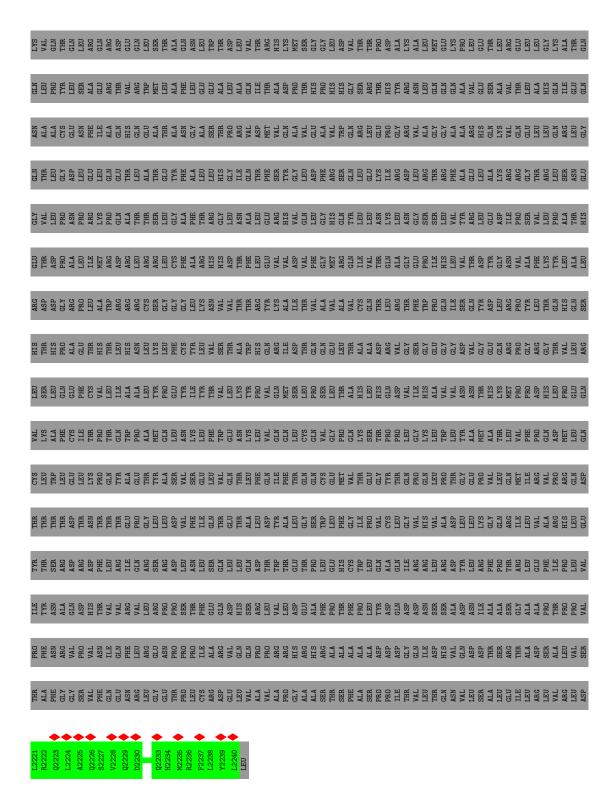
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 Chain h: • Molecule 1: Triplex capsid protein 2 Chain I: 98% • Molecule 1: Triplex capsid protein 2 Chain n: 95% • Molecule 1: Triplex capsid protein 2 Chain o: 94% 6% • Molecule 2: Large tegument protein deneddylase Chain H: THE PROPERTY OF THE PROPERTY O



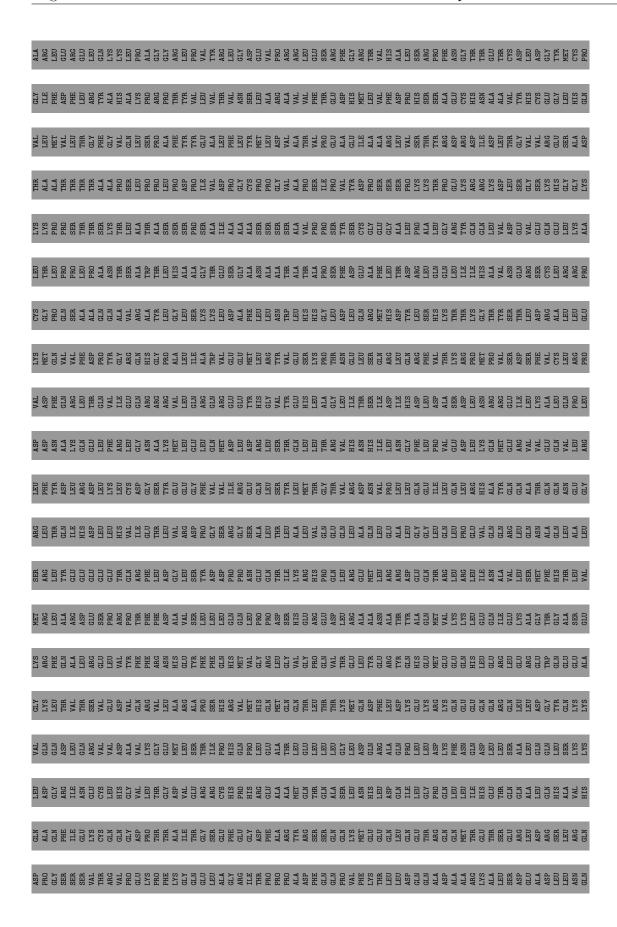




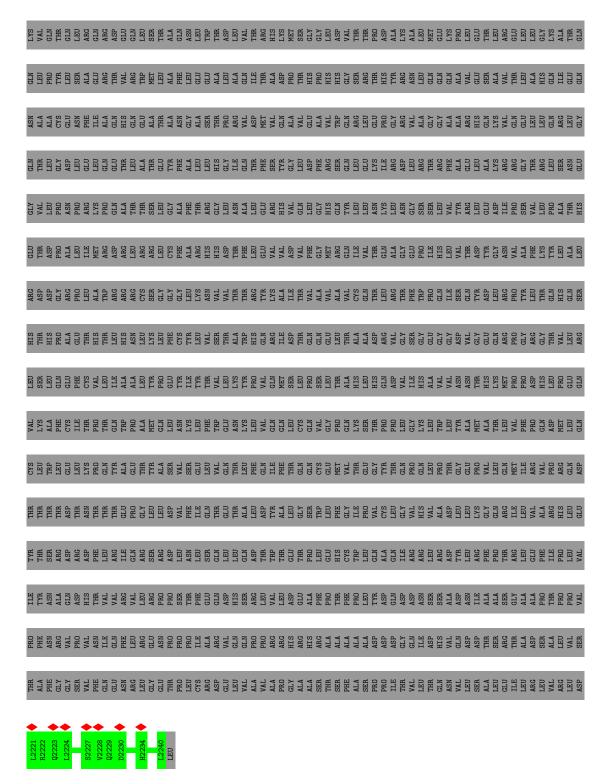


• Molecule 2: Large tegument protein deneddylase







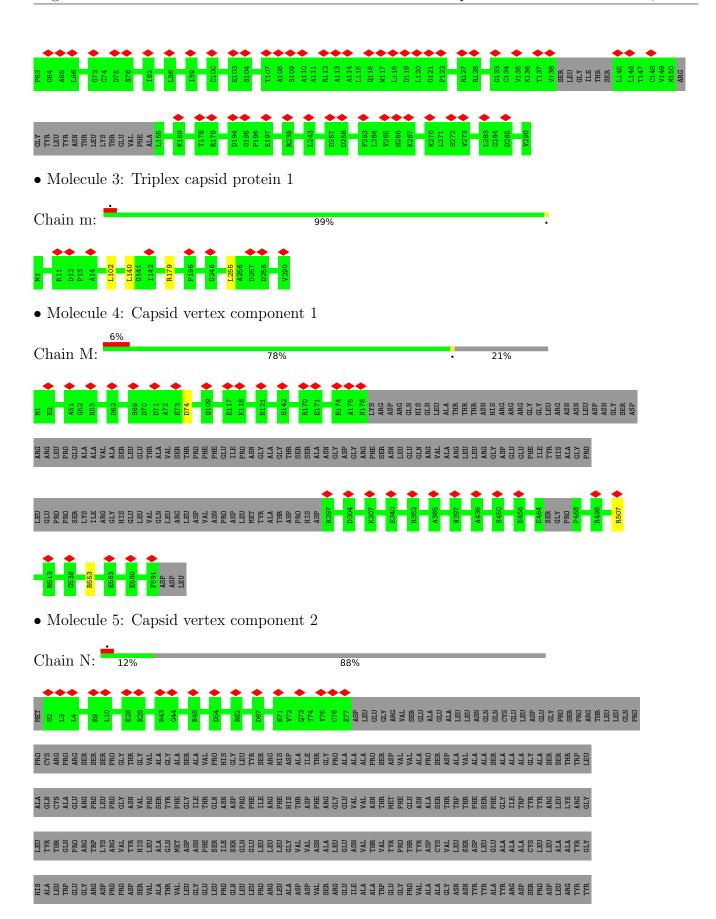


• Molecule 3: Triplex capsid protein 1

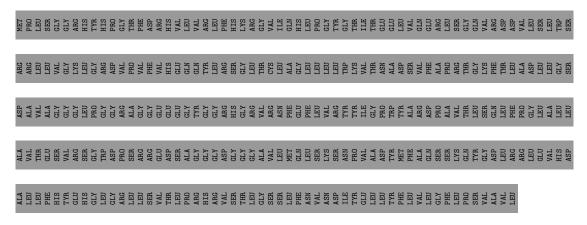
Chain g: 78% 22%



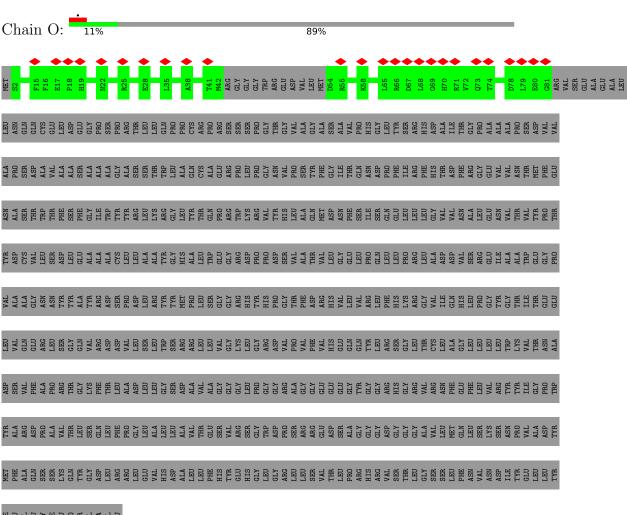








• Molecule 5: Capsid vertex component 2



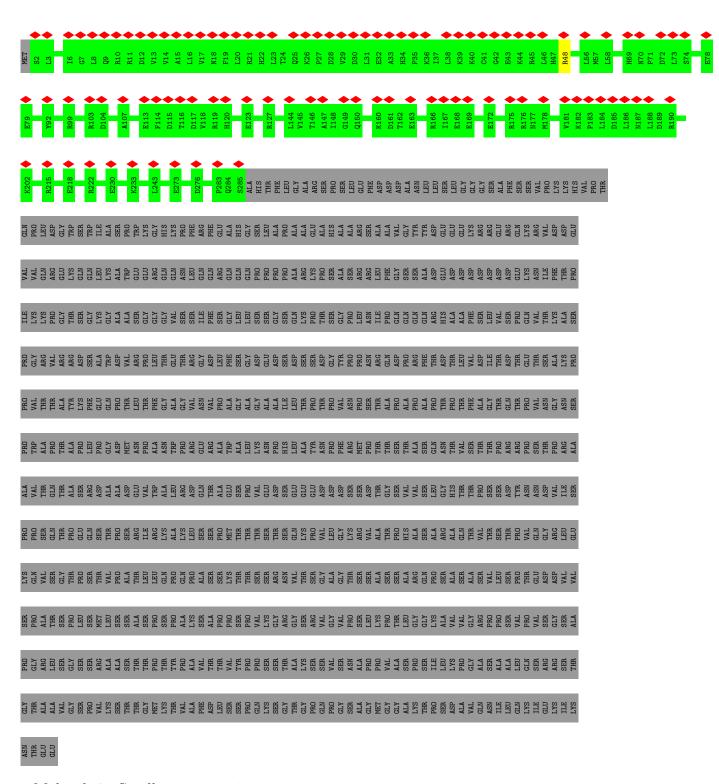
PHE LEU VAL LEU GLY PHE LEU PRO SER VAL ALA

• Molecule 6: ORFL92C UL32

10%

Chain 1: 27% 73%

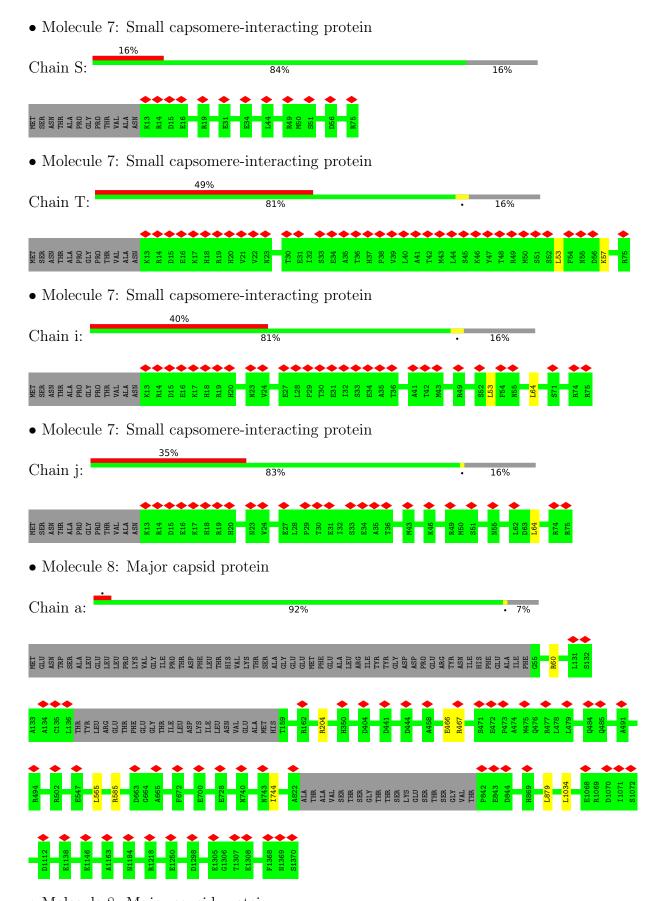




• Molecule 7: Small capsomere-interacting protein

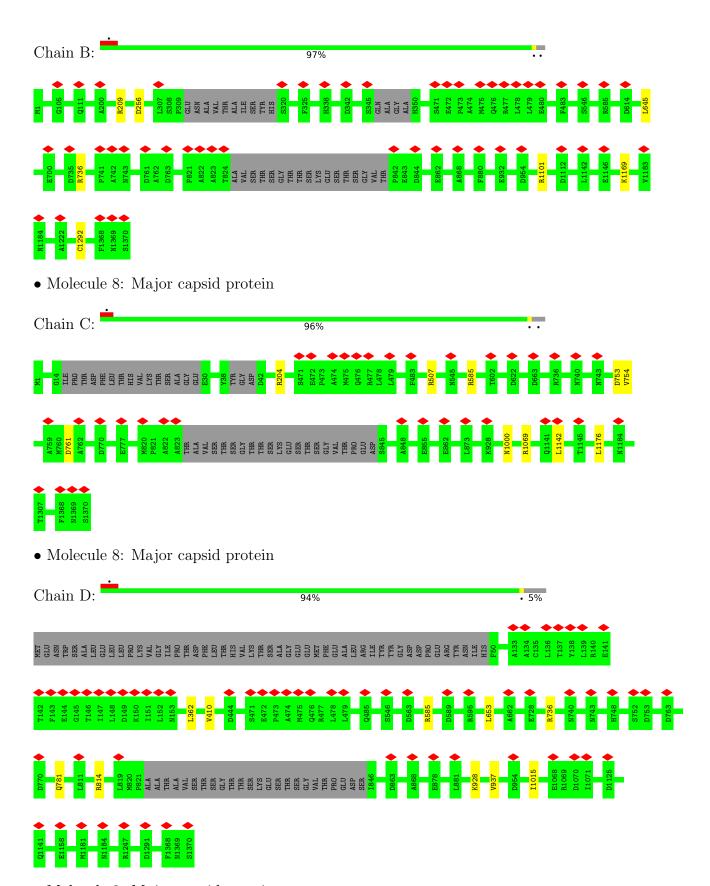
Chain R: 84% 16%





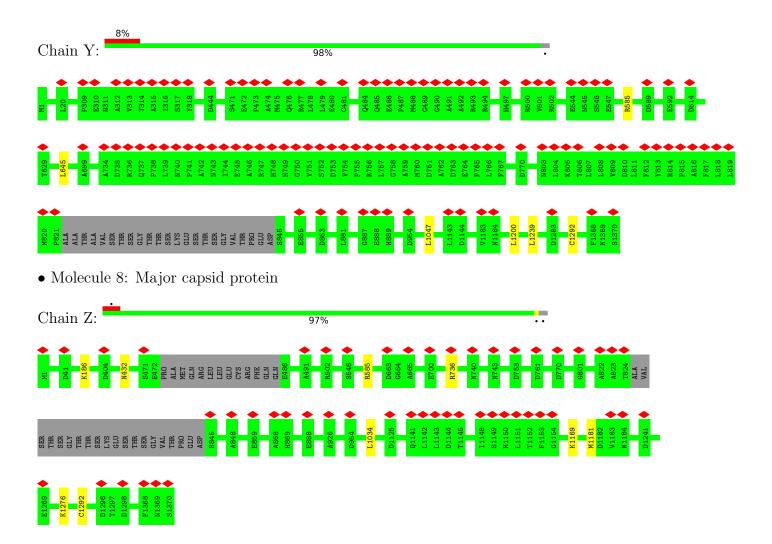
• Molecule 8: Major capsid protein





• Molecule 8: Major capsid protein







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	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	0.093	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	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	Е	Bond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	I	0.31	0/2436	0.65	2/3310 (0.1%)
1	h	0.31	0/2431	0.58	0/3306
1	n	0.30	0/2374	0.52	0/3225
1	О	0.30	0/2333	0.51	0/3167
2	Н	0.27	0/174	0.60	0/233
2	Р	0.28	0/174	0.51	0/233
3	g	0.31	0/1860	0.57	0/2521
3	m	0.34	0/2374	0.58	2/3221 (0.1%)
4	M	0.34	0/3935	0.57	0/5331
5	N	0.30	0/662	0.62	0/892
5	О	0.27	0/600	0.58	0/808
6	1	0.28	0/2358	0.55	0/3182
7	R	0.28	0/520	0.59	0/697
7	S	0.31	0/520	0.59	0/697
7	Т	0.27	0/520	0.62	1/697~(0.1%)
7	i	0.29	0/520	0.74	2/697~(0.3%)
7	j	0.30	0/520	0.64	0/697
8	В	0.34	0/10870	0.58	2/14804 (0.0%)
8	С	0.34	0/10786	0.57	3/14692 (0.0%)
8	D	0.33	0/10513	0.54	$1/14322 \ (0.0\%)$
8	Y	0.32	0/10932	0.54	3/14892 (0.0%)
8	Z	0.33	0/10835	0.54	$1/14762 \ (0.0\%)$
8	a	0.34	0/10318	0.57	3/14057 (0.0%)
All	All	0.33	0/88565	0.56	20/120443 (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 maintenain group or atoms of a sidechain that are expected to be planar.

\mathbf{Mol}	Chain	#Chirality outliers	#Planarity outliers
8	С	0	1
8	D	0	1



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Mol	Chain	#Chirality outliers	#Planarity outliers
8	Y	0	1
8	Z	0	1
8	a	0	1
All	All	0	5

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
8	С	1142	LEU	CA-CB-CG	8.64	135.16	115.30
1	I	179	ASP	CB-CG-OD2	8.31	125.78	118.30
3	m	140	LEU	CA-CB-CG	6.81	130.96	115.30
7	i	64	LEU	CA-CB-CG	6.66	130.63	115.30
8	С	761	ASP	CB-CG-OD2	6.65	124.28	118.30
8	В	645	LEU	CA-CB-CG	6.27	129.72	115.30
8	Y	1239	LEU	CA-CB-CG	5.95	128.99	115.30
8	С	1176	LEU	CA-CB-CG	5.93	128.94	115.30
7	Т	53	LEU	CA-CB-CG	5.82	128.69	115.30
7	i	53	LEU	CA-CB-CG	5.71	128.43	115.30
8	В	1292	CYS	CA-CB-SG	5.71	124.28	114.00
8	a	744	ILE	CG1-CB-CG2	-5.67	98.93	111.40
3	m	255	LEU	CA-CB-CG	5.25	127.37	115.30
8	Y	645	LEU	CA-CB-CG	5.19	127.23	115.30
8	Y	1047	LEU	CA-CB-CG	5.15	127.14	115.30
8	D	362	LEU	CA-CB-CG	5.14	127.13	115.30
1	I	202	LEU	CA-CB-CG	5.13	127.11	115.30
8	Z	1034	LEU	CA-CB-CG	5.10	127.03	115.30
8	a	879	LEU	CA-CB-CG	5.07	126.96	115.30
8	a	1034	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	С	585	ARG	Peptide
8	D	585	ARG	Peptide
8	Y	585	ARG	Peptide
8	Z	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 (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	Perce	ntiles
1	I	299/306~(98%)	287 (96%)	12 (4%)	0	100	100
1	h	298/306~(97%)	283 (95%)	15 (5%)	0	100	100
1	n	290/306~(95%)	273 (94%)	17 (6%)	0	100	100
1	О	285/306~(93%)	274 (96%)	11 (4%)	0	100	100
2	Н	18/2241 (1%)	18 (100%)	0	0	100	100
2	P	18/2241 (1%)	18 (100%)	0	0	100	100
3	g	221/290 (76%)	204 (92%)	17 (8%)	0	100	100
3	m	288/290 (99%)	274 (95%)	14 (5%)	0	100	100
4	M	462/594 (78%)	442 (96%)	20 (4%)	0	100	100
5	N	74/642 (12%)	70 (95%)	4 (5%)	0	100	100
5	О	65/642 (10%)	64 (98%)	1 (2%)	0	100	100
6	1	282/1048 (27%)	269 (95%)	13 (5%)	0	100	100
7	R	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	S	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	Т	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
7	i	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
7	j	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
8	В	1331/1370 (97%)	1260 (95%)	71 (5%)	0	100	100
8	С	1323/1370 (97%)	1268 (96%)	55 (4%)	0	100	100
8	D	1293/1370 (94%)	1210 (94%)	83 (6%)	0	100	100
8	Y	1343/1370 (98%)	1267 (94%)	76 (6%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percer	ntiles
8	Z	1331/1370 (97%)	1264 (95%)	67 (5%)	0	100	100
8	a	1269/1370 (93%)	1216 (96%)	53 (4%)	0	100	100
All	All	10795/17807 (61%)	10256 (95%)	539 (5%)	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	Perce	ntiles
1	I	$270/273\ (99\%)$	270 (100%)	0	100	100
1	h	$270/273\ (99\%)$	270 (100%)	0	100	100
1	n	263/273 (96%)	260 (99%)	3 (1%)	73	85
1	О	$259/273\ (95\%)$	258 (100%)	1 (0%)	91	94
2	Н	19/1941 (1%)	19 (100%)	0	100	100
2	Р	19/1941~(1%)	19 (100%)	0	100	100
3	g	199/252 (79%)	198 (100%)	1 (0%)	88	93
3	m	$252/252 \ (100\%)$	250 (99%)	2 (1%)	81	89
4	M	395/500 (79%)	392 (99%)	3 (1%)	81	89
5	N	69/526~(13%)	69 (100%)	0	100	100
5	О	64/526 (12%)	64 (100%)	0	100	100
6	1	255/883 (29%)	254 (100%)	1 (0%)	91	94
7	R	59/68 (87%)	59 (100%)	0	100	100
7	S	59/68 (87%)	59 (100%)	0	100	100
7	Т	59/68 (87%)	58 (98%)	1 (2%)	60	78
7	i	59/68 (87%)	59 (100%)	0	100	100
7	j	59/68 (87%)	58 (98%)	1 (2%)	60	78
8	В	1169/1192 (98%)	1164 (100%)	5 (0%)	91	94
8	С	1156/1192 (97%)	1150 (100%)	6 (0%)	88	93



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
8	D	$1130/1192\ (95\%)$	1122 (99%)	8 (1%)	84	90
8	Y	1174/1192 (98%)	1172 (100%)	2 (0%)	93	96
8	Z	1163/1192 (98%)	1156 (99%)	7 (1%)	86	92
8	a	1110/1192 (93%)	1105 (100%)	5 (0%)	88	93
All	All	9531/15405 (62%)	9485 (100%)	46 (0%)	89	93

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

Mol	Chain	Res	Type
1	n	176	THR
1	n	201	CYS
1	n	303	ILE
1	О	37	ARG
3	g	49	ARG
3	m	102	LEU
3	m	179	ARG
4	M	74	ASP
4	M	507	ARG
4	M	553	ARG
6	1	48	ARG
7	Т	57	LYS
7	j	64	LEU
8	a	60	ARG
8	a	204	ARG
8	a	466	GLU
8	a	467	ARG
8	a	565	LEU
8	В	209	ARG
8	В	256	ASP
8	В	736	ARG
8	В	1101	ARG
8	В	1169	LYS
8	С	204	ARG
8	С	507	ARG
8	С	753	ASP
8	C	754	VAL
8	С	1000	ASN
8	С	1069	ARG
8	D	410	VAL
8	D	653	LEU
8	D	736	ARG



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Mol	Chain	Res	Type
8	D	781	GLN
8	D	814	ARG
8	D	928	LYS
8	D	937	VAL
8	D	1015	ILE
8	Y	1200	LEU
8	Y	1292	CYS
8	Z	186	LYS
8	Z	432	ASN
8	Z	736	ARG
8	Z	1169	LYS
8	Z	1181	MET
8	Z	1276	LYS
8	Z	1292	CYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such side chains are listed below:

Mol	Chain	Res	Type
1	h	14	HIS
1	h	36	GLN
1	h	123	ASN
1	h	277	GLN
1	h	297	ASN
1	I	43	HIS
1	I	79	ASN
1	I	173	GLN
1	I	235	GLN
1	I	258	HIS
1	I	277	GLN
2	Н	2234	HIS
2	Р	2233	GLN
1	n	43	HIS
1	n	50	GLN
1	n	277	GLN
1	О	7	ASN
1	О	209	ASN
3	g	249	GLN
3	m	116	GLN
3	m	266	HIS
4	M	47	ASN
4	M	145	GLN
4	M	333	ASN



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Mol	Chain	Res	Type
4	M	560	GLN
5	N	5	HIS
5	N	73	GLN
5	О	22	ASN
5	О	63	GLN
6	1	18	ASN
6	1	70	ASN
6	1	120	HIS
6	1	150	GLN
6	1	158	HIS
6	1	170	ASN
6	1	201	ASN
6	1	248	ASN
7	R	18	HIS
7	R	37	HIS
7	Т	37	HIS
7	j	20	HIS
8	a	111	GLN
8	a	338	HIS
8	a	378	ASN
8	a	485	GLN
8	a	510	ASN
8	a	534	HIS
8	a	649	HIS
8	a	731	GLN
8	a	849	GLN
8	a	903	GLN
8	a	945	ASN
8	a	1000	ASN
8	a	1080	ASN
8	a	1190	ASN
8	a	1191	ASN
8	a	1230	ASN
8	a	1245	ASN
8	a	1350	HIS
8	В	76	HIS
8	В	214	ASN
8	В	231	ASN
8	В	388	ASN
8	В	438	GLN
8	В	534	HIS
8	В	543	GLN

8 | B | 543 | GLN | Continued on next page...



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Continued from previous page			
Mol	Chain	Res	Type
8	В	711	HIS
8	В	740	ASN
8	В	749	HIS
8	В	849	GLN
8	В	914	GLN
8	В	985	ASN
8	В	1000	ASN
8	В	1023	GLN
8	В	1027	HIS
8	В	1029	HIS
8	В	1061	ASN
8	В	1160	ASN
8	В	1166	HIS
8	В	1319	GLN
8	В	1369	ASN
8	B C C C C C C C C C C C C C C C C C C C	166	ASN
8	С	214	ASN
8	С	462	GLN
8	С	484	GLN
8	С	510	ASN
8	С	534	HIS
8	С	620	ASN
8	С	695	ASN GLN
8	С	874	
8	С	901	HIS
8	С	914	GLN
8	С	985	ASN
8		1029	HIS
8	С	1079	GLN
8	С	1184	ASN
8	С	1264	GLN
8	С	1319	GLN
8	C C C D	1363	GLN
8		96	GLN
8	D	111	GLN
8	D	153	ASN
8	D	214	ASN
8	D	326	ASN
8	D	346	GLN
8	D	371	ASN
8	D	510	ASN
8	D	543	GLN

8 D 543 GLN

Continued on next page...



Continued from previous page

Mol Chain Res Type 8 D 560 ASN 8 D 571 HIS 8 D 620 ASN 8 D 673 HIS 8 D 794 ASN 8 D 795 ASN 8 D 1000 ASN 8 D 1061 ASN 8 D 1061 ASN 8 D 1079 GLN 8 D 1166 HIS 8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 281 GLN 8 Y 534 HIS 8 Y 708 ASN 8 Y	Continued from previous page			
8 D 571 HIS 8 D 620 ASN 8 D 673 HIS 8 D 794 ASN 8 D 795 ASN 8 D 919 ASN 8 D 1000 ASN 8 D 1061 ASN 8 D 1079 GLN 8 D 1166 HIS 8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 795 ASN 8 Y 795 ASN 8 Y <td< th=""><th></th><th>Chain</th><th>Res</th><th>Type</th></td<>		Chain	Res	Type
8 D 620 ASN 8 D 673 HIS 8 D 794 ASN 8 D 795 ASN 8 D 919 ASN 8 D 1000 ASN 8 D 1061 ASN 8 D 1079 GLN 8 D 1120 ASN 8 D 1360 HIS 8 D 1369 ASN 8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y <t< td=""><td></td><td></td><td></td><td></td></t<>				
8 D 673 HIS 8 D 794 ASN 8 D 795 ASN 8 D 919 ASN 8 D 1000 ASN 8 D 1061 ASN 8 D 1079 GLN 8 D 1120 ASN 8 D 1360 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 534 HIS 8 Y 534 HIS 8 Y 795 ASN 8 Y 940 HIS 8 Y 940 HIS 8 Y <td< td=""><td></td><td></td><td></td><td></td></td<>				
8 D 794 ASN 8 D 795 ASN 8 D 919 ASN 8 D 1000 ASN 8 D 1061 ASN 8 D 1079 GLN 8 D 1120 ASN 8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 153 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 1080 ASN 8 Y <t< td=""><td></td><td></td><td></td><td></td></t<>				
8 D 795 ASN 8 D 919 ASN 8 D 1000 ASN 8 D 1061 ASN 8 D 1079 GLN 8 D 1120 ASN 8 D 1166 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 940 HIS 8 Y 1029 HIS 8 Y <t< td=""><td></td><td>D</td><td></td><td></td></t<>		D		
8 D 919 ASN 8 D 1000 ASN 8 D 1061 ASN 8 D 1079 GLN 8 D 1120 ASN 8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 153 ASN 8 Y 153 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y <	8		794	ASN
8 D 1000 ASN 8 D 1061 ASN 8 D 1079 GLN 8 D 1120 ASN 8 D 1166 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1080 ASN 8 Y			795	
8 D 1079 GLN 8 D 1120 ASN 8 D 1166 HIS 8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 510 ASN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z	8		919	
8 D 1079 GLN 8 D 1120 ASN 8 D 1166 HIS 8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 199 ASN 8 Y 510 ASN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z	8		1000	ASN
8 D 1120 ASN 8 D 1166 HIS 8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8	8	D	1061	
8 D 1120 ASN 8 D 1166 HIS 8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8	8	D	1079	GLN
8 D 1350 HIS 8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 940 HIS 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 388 ASN 8 Z 497 HIS 8	8	D	1120	ASN
8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 914 GLN 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z	8		1166	HIS
8 D 1369 ASN 8 Y 153 ASN 8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 914 GLN 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z	8	D	1350	HIS
8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 914 GLN 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN	8	D	1369	ASN
8 Y 199 ASN 8 Y 281 GLN 8 Y 510 ASN 8 Y 534 HIS 8 Y 708 ASN 8 Y 795 ASN 8 Y 914 GLN 8 Y 940 HIS 8 Y 981 HIS 8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN	8	Y	153	ASN
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN	8	Y		ASN
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y	281	
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1029 HIS 8 Y 1080 ASN 8 Y 1160 ASN 8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1264 GLN 8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Y 1350 HIS 8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Z 76 HIS 8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN		Y		
8 Z 181 GLN 8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN				
8 Z 257 ASN 8 Z 388 ASN 8 Z 497 HIS 8 Z 514 GLN				
8 Z 514 GLN		$\frac{Z}{Z}$		
8 Z 514 GLN		$\frac{2}{7}$		
8 Z 514 GLN		$\frac{Z}{Z}$		
8 Z 543 GLN		<u>Z</u>		
		7		
8 Z 660 HIS		<u>Z</u>		
8 Z 697 GLN		<u> </u>		
8 Z 697 GLN 8 Z 901 HIS 8 Z 919 ASN		7.		
8 Z 919 ASN		<u> </u>		
8 Z 984 HIS	8	<u> </u>		
8 Z 1060 ASN		7.		
Continued on next page	U			



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Mol	Chain	Res	Type
8	Z	1082	ASN
8	Z	1223	GLN
8	Z	1230	ASN
8	Z	1264	GLN
8	Z	1313	ASN
8	Z	1363	GLN
8	Z	1364	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 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.



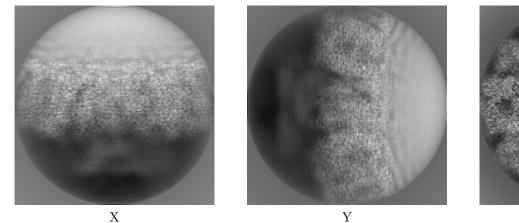
6 Map visualisation (i)

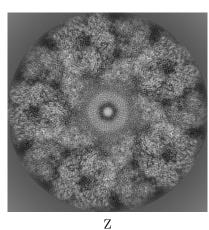
This section contains visualisations of the EMDB entry EMD-31298. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

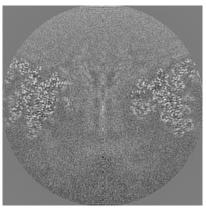




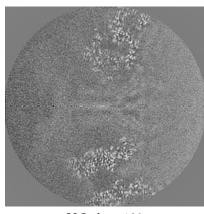
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

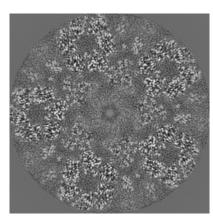
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

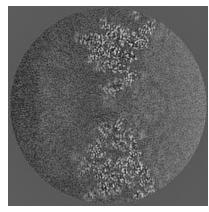


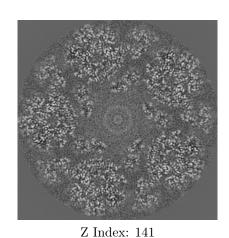
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map







X Index: 116 Y Index: 97

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







The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

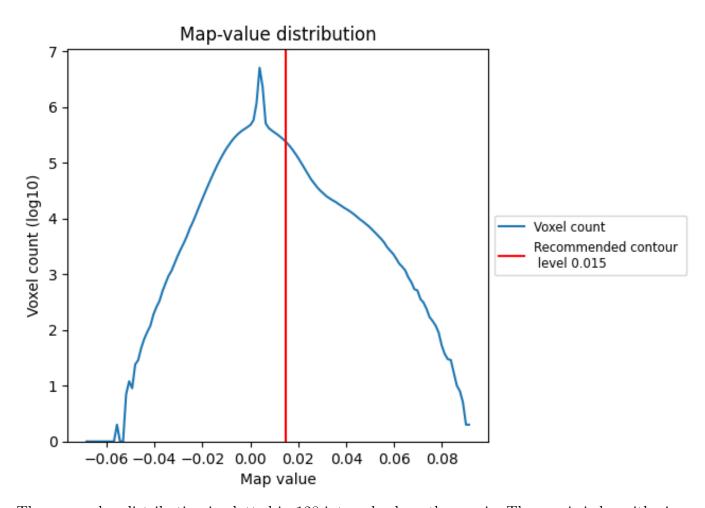
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

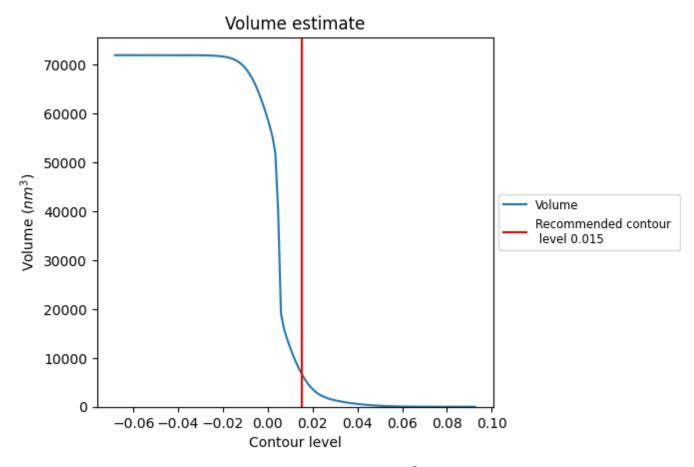
7.1 Map-value distribution (i)



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)

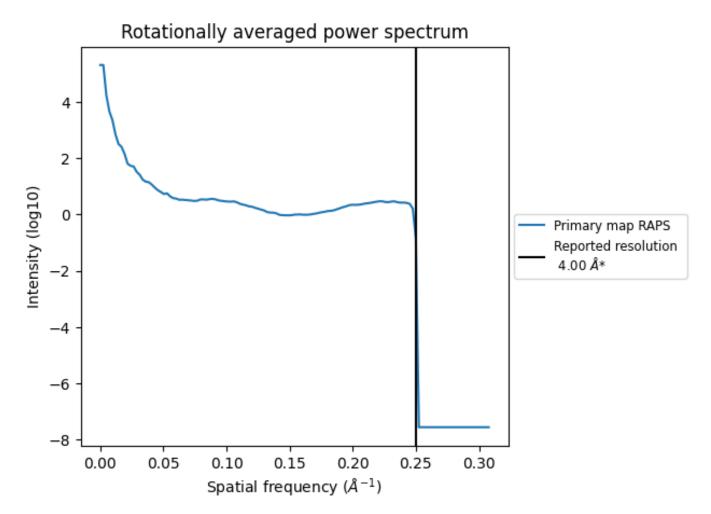


The volume at the recommended contour level is $6849~\mathrm{nm}^3$; this corresponds to an approximate mass of $6187~\mathrm{kDa}$.

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 $\rm \mathring{A}^{-1}$



8 Fourier-Shell correlation (i)

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

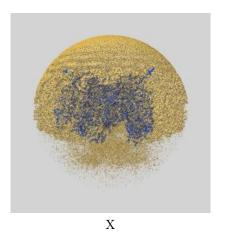


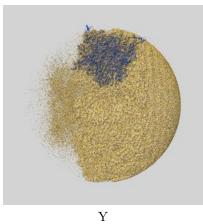
9 Map-model fit (i)

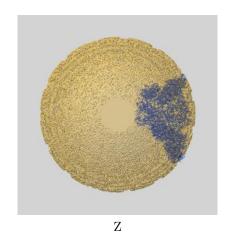
This section contains information regarding the fit between EMDB map EMD-31298 and PDB model 7ETJ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

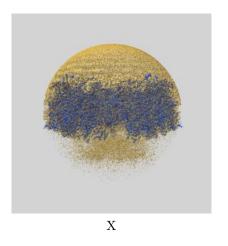
9.1.1 Map-model overlay (i)

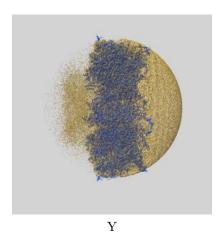


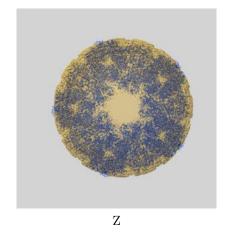




9.1.2 Map-model assembly overlay (i)



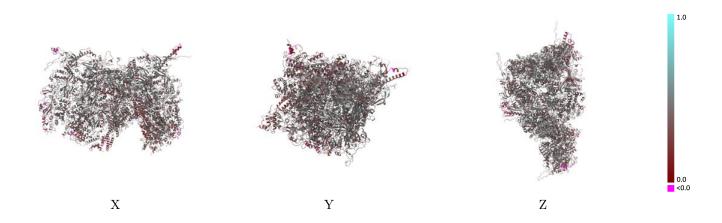




The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

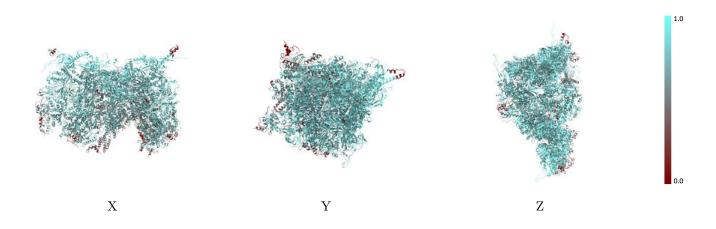


9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according 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.

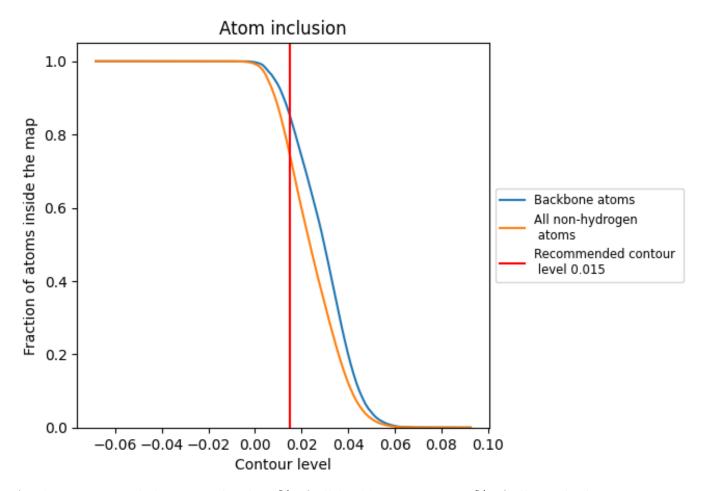
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).



9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7435	0.4060
1	0.5073	0.3130
В	0.7709	0.4180
С	0.7895	0.4290
D	0.7805	0.4160
Н	0.4132	0.2030
I	0.6933	0.3800
M	0.7212	0.4020
N	0.6100	0.3640
О	0.5018	0.2500
Р	0.5329	0.2810
R	0.5060	0.3210
S	0.5964	0.3500
Т	0.3032	0.2460
Y	0.7567	0.4060
Z	0.7865	0.4280
a	0.7768	0.4250
g	0.5517	0.3090
h	0.6854	0.3930
i	0.3855	0.2820
j	0.4478	0.3160
m	0.7788	0.4300
n	0.7739	0.4140
0	0.7692	0.4100



