



## Full wwPDB EM Validation Report ⓘ

Dec 30, 2024 – 09:29 PM EST

PDB ID : 8FJL  
EMDB ID : EMD-29244  
Title : Golden Shiner Reovirus Core Tropical Vertex  
Authors : Stevens, A.S.; Zhou, Z.H.  
Deposited on : 2022-12-19  
Resolution : 3.27 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>.

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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) : 2.40

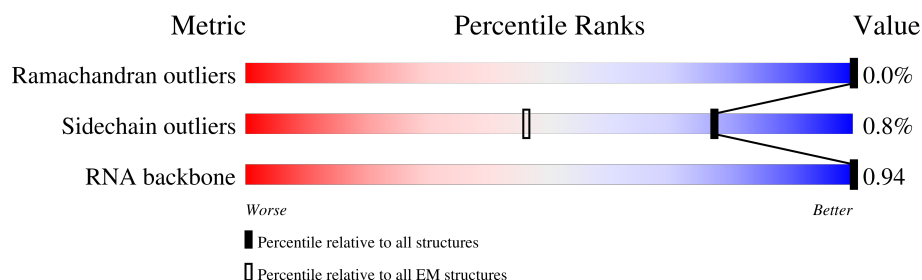
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.27 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.



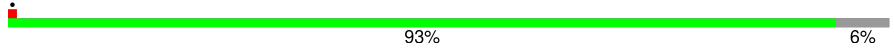
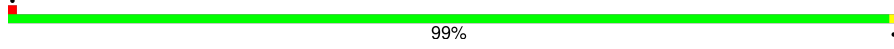
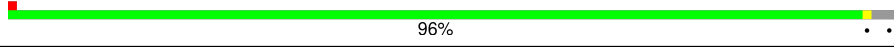
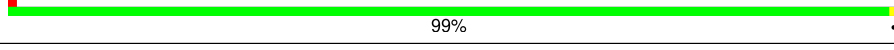
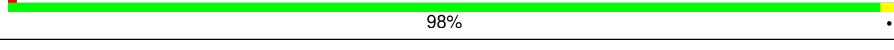
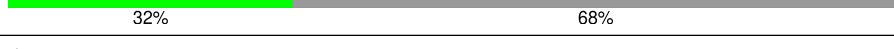

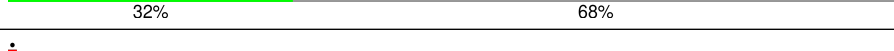
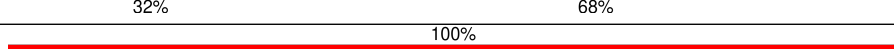
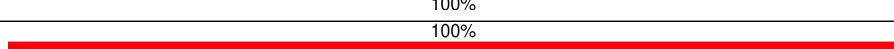
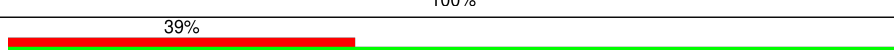
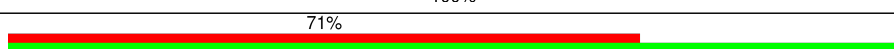

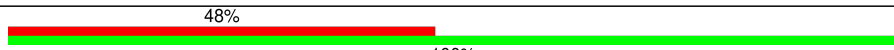


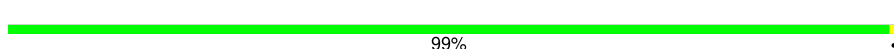

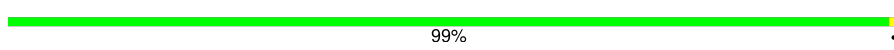
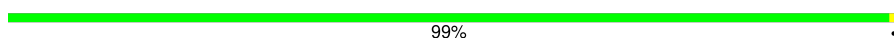
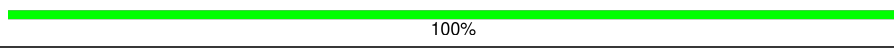
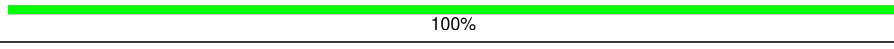
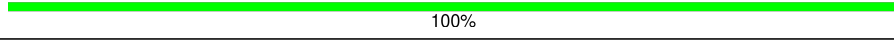
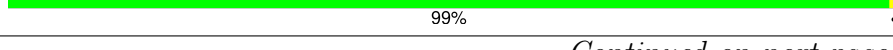

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	1273	
2	B	718	
3	C	1138	
3	D	1138	
3	E	1138	
3	F	1138	
3	G	1138	
3	H	1138	

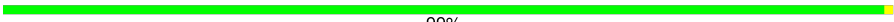






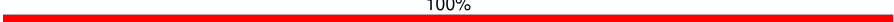

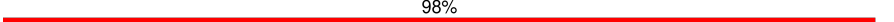
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Mol	Chain	Length	Quality of chain
3	I	1138	
3	J	1138	
3	K	1138	
3	L	1138	
4	M	94	
4	N	94	
4	k	94	
4	l	94	
4	m	94	
5	a5	28	
5	b5	28	
6	a6	38	
6	b6	38	
7	a1	52	
7	b1	52	
8	a3	40	
8	b3	40	
9	V	411	
9	W	411	
9	X	411	
9	a	411	
9	b	411	
9	d	411	
9	e	411	
9	g	411	

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Mol	Chain	Length	Quality of chain
9	h	411	 99% .
9	n	411	 100%
10	Y	1297	 99% .
10	Z	1297	 99% .
10	c	1297	 99% .
10	f	1297	 99% .
10	i	1297	 99% .
11	a2	60	 100%
11	b2	60	 98%
11			 100%

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 197669 atoms, of which 4598 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 RNA-directed RNA polymerase VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1273	Total	C	N	O	S	0	0
			9978	6375	1736	1822	45		

- Molecule 2 is a protein called Microtubule-associated protein VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	718	Total	C	N	O	S	0	0
			5593	3588	971	1016	18		

- Molecule 3 is a protein called Major inner capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1075	Total	C	N	O	S	0	0
			8300	5296	1421	1534	49		
3	D	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		
3	E	1106	Total	C	N	O	S	0	0
			8534	5440	1463	1579	52		
3	F	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		
3	G	1098	Total	C	N	O	S	0	0
			8477	5403	1454	1568	52		
3	H	1130	Total	C	N	O	S	0	0
			8699	5540	1491	1615	53		
3	I	1065	Total	C	N	O	S	0	0
			8226	5244	1412	1519	51		
3	J	1130	Total	C	N	O	S	0	0
			8696	5537	1491	1615	53		
3	K	1098	Total	C	N	O	S	0	0
			8477	5403	1454	1568	52		
3	L	1138	Total	C	N	O	S	0	0
			8761	5578	1502	1628	53		

- Molecule 4 is a protein called Major inner capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	94	Total	C	N	O	S	0	0
			640	377	113	149	1		
4	N	30	Total	C	N	O	S	0	0
			210	128	36	45	1		
4	k	30	Total	C	N	O	S	0	0
			211	128	36	46	1		
4	l	30	Total	C	N	O	S	0	0
			211	128	36	46	1		
4	m	30	Total	C	N	O	S	0	0
			211	128	36	46	1		

- Molecule 5 is a RNA chain called RNA (38-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	a5	28	Total 881	C 266	H 296	N 98	O 194	P 27	0	0
5	b5	28	Total 881	C 266	H 296	N 98	O 194	P 27	0	0

- Molecule 6 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	b6	38	Total 1196	C 361	H 401	N 133	O 264	P 37	0	0
6	a6	38	Total 1196	C 361	H 401	N 133	O 264	P 37	0	0

- Molecule 7 is a RNA chain called RNA (52-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	a1	52	Total 1637	C 494	H 548	N 182	O 362	P 51	0	0
7	b1	52	Total 1637	C 494	H 548	N 182	O 362	P 51	0	0

- Molecule 8 is a RNA chain called RNA (39-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	a3	40	Total 1259	C 380	H 422	N 140	O 278	P 39	0	0
8	b3	40	Total 1259	C 380	H 422	N 140	O 278	P 39	0	0

- Molecule 9 is a protein called Clamp protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	W	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	X	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	a	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	b	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	d	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	e	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	g	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	h	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		
9	n	411	Total	C	N	O	S	0	0
			3138	2008	544	570	16		

- Molecule 10 is a protein called Outer capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
10	Z	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
10	c	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
10	f	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		
10	i	1297	Total	C	N	O	S	0	0
			9963	6382	1694	1860	27		

- Molecule 11 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
11	a2	60	Total	C	H	N	O	P	0	0
			1889	570	632	210	418	59		
11	b2	60	Total	C	H	N	O	P	0	0
			1889	570	632	210	418	59		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

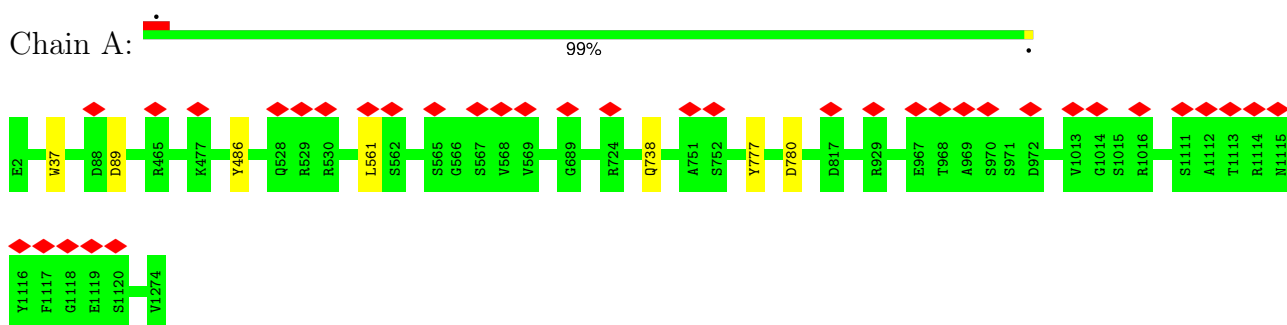
Mol	Chain	Residues	Atoms		AltConf
12	E	1	Total 1	Zn 1	0
12	G	1	Total 1	Zn 1	0
12	I	1	Total 1	Zn 1	0
12	K	1	Total 1	Zn 1	0



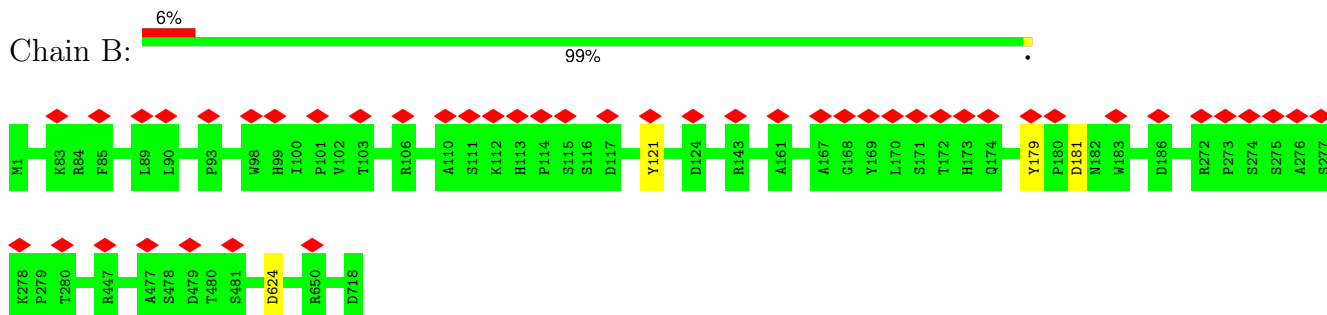
### 3 Residue-property plots

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.

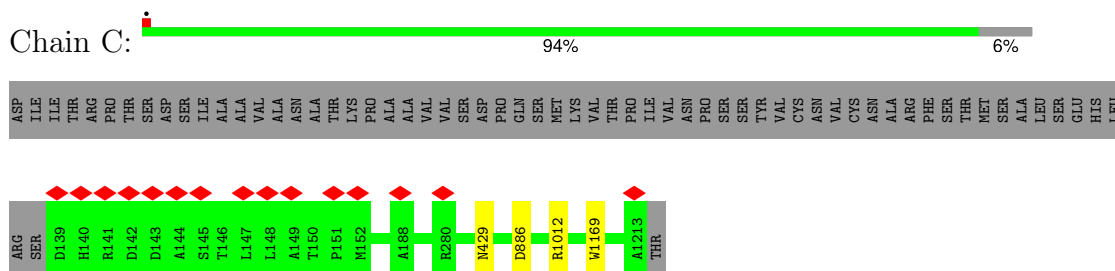
- Molecule 1: RNA-directed RNA polymerase VP2



- Molecule 2: Microtubule-associated protein VP5

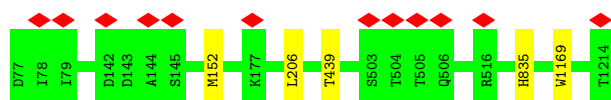


- Molecule 3: Major inner capsid protein VP3



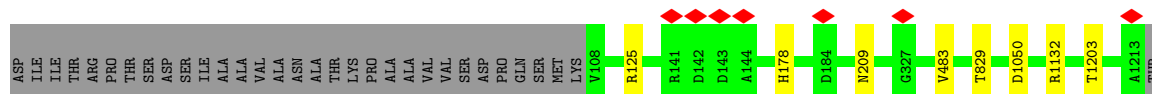
- Molecule 3: Major inner capsid protein VP3





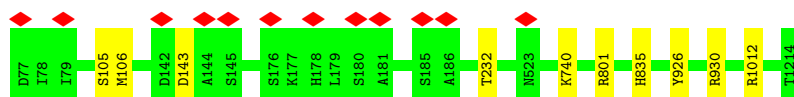
- Molecule 3: Major inner capsid protein VP3

Chain E: 96%



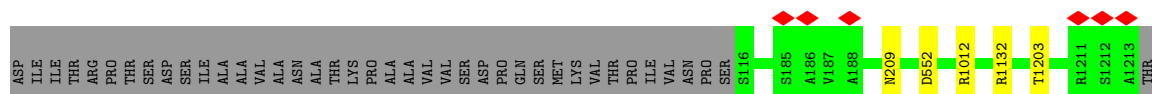
- Molecule 3: Major inner capsid protein VP3

Chain F: 99%



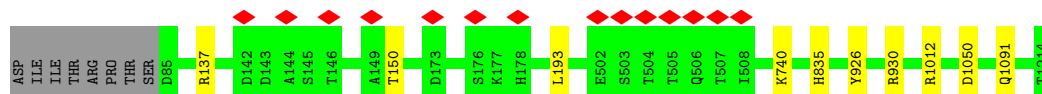
- Molecule 3: Major inner capsid protein VP3

Chain G: 96%



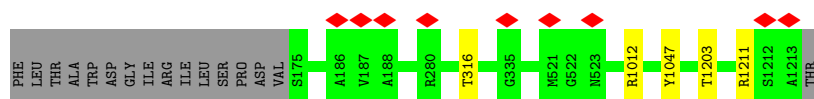
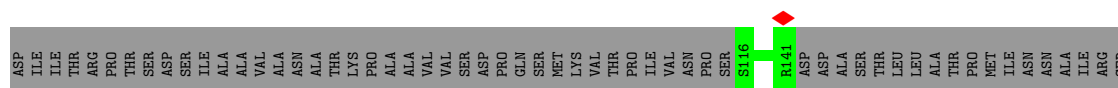
- Molecule 3: Major inner capsid protein VP3

Chain H: 98%



- Molecule 3: Major inner capsid protein VP3

Chain I: 93% 6%

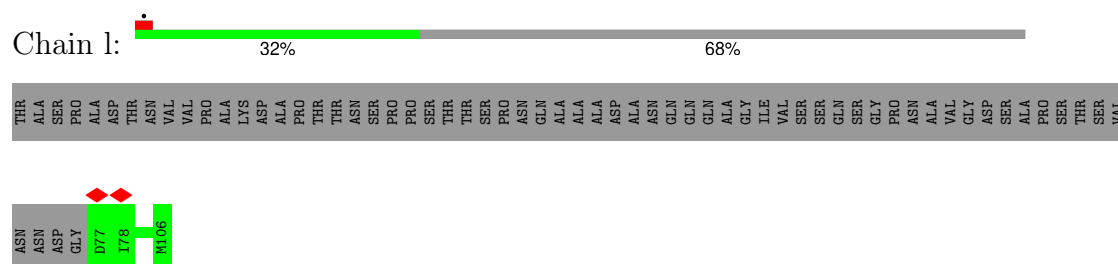


- Molecule 3: Major inner capsid protein VP3

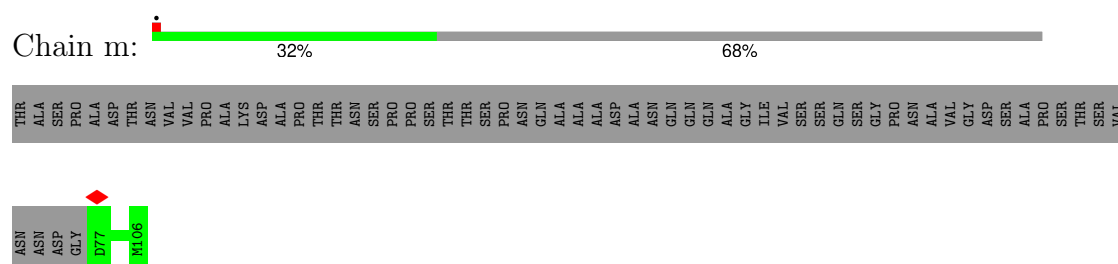
Chain J: 99%



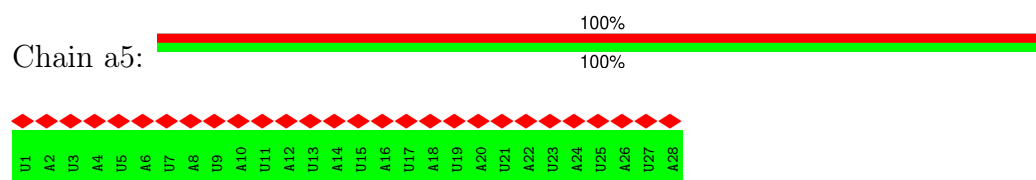
- Molecule 4: Major inner capsid protein VP3



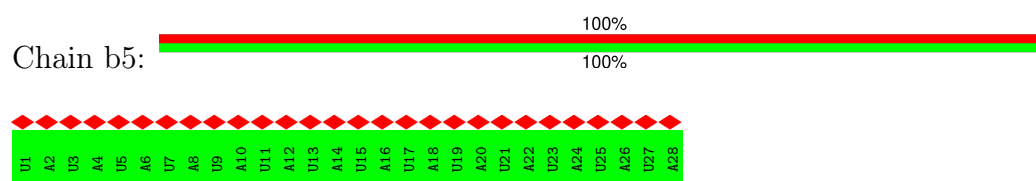
- Molecule 4: Major inner capsid protein VP3



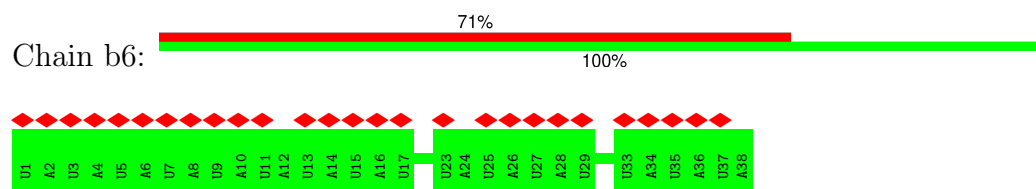
- Molecule 5: RNA (38-MER)



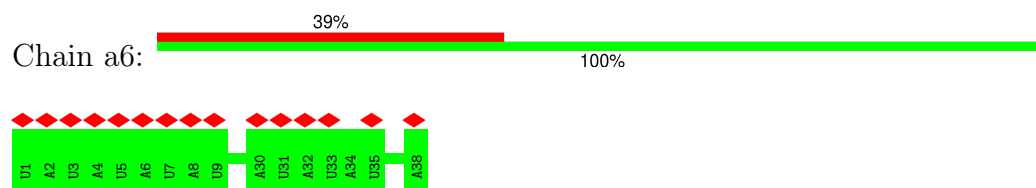
- Molecule 5: RNA (38-MER)



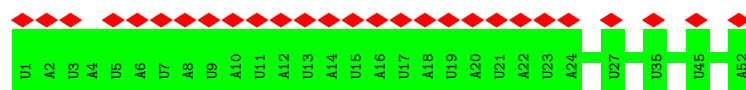
- Molecule 6: RNA (30-MER)



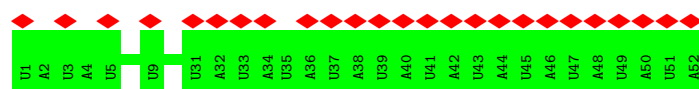
- Molecule 6: RNA (30-MER)



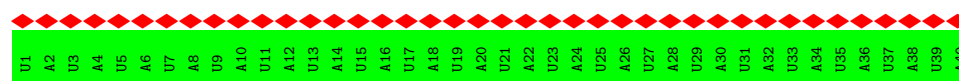
## • Molecule 7: RNA (52-MER)



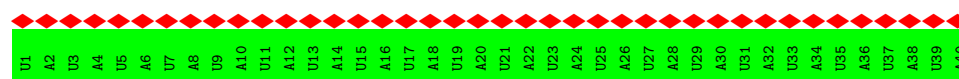
## • Molecule 7: RNA (52-MER)



## • Molecule 8: RNA (39-MER)



## • Molecule 8: RNA (39-MER)



## • Molecule 9: Clamp protein VP6



## • Molecule 9: Clamp protein VP6

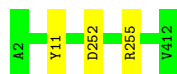


## • Molecule 9: Clamp protein VP6



- Molecule 9: Clamp protein VP6

Chain a:  99%



- Molecule 9: Clamp protein VP6

Chain b:  100%



- Molecule 9: Clamp protein VP6

Chain d:  100%



- Molecule 9: Clamp protein VP6

Chain e:  100%



- Molecule 9: Clamp protein VP6

Chain g:  99%



- Molecule 9: Clamp protein VP6

Chain h:  99%



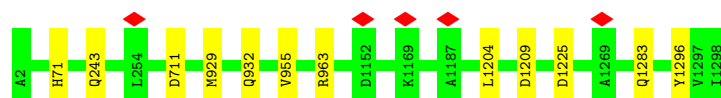
- Molecule 9: Clamp protein VP6

Chain n:  100%



- Molecule 10: Outer capsid protein VP1

Chain Y:  99%



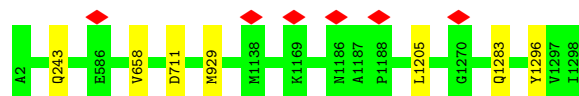
- Molecule 10: Outer capsid protein VP1

Chain Z:  99%



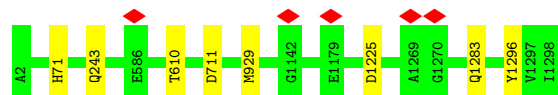
- Molecule 10: Outer capsid protein VP1

Chain c:  99%



- Molecule 10: Outer capsid protein VP1

Chain f:  99%



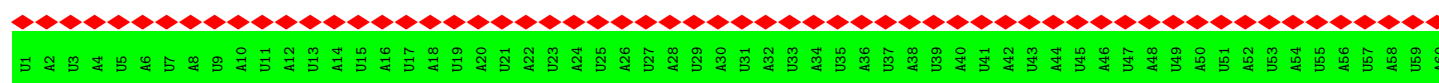
- Molecule 10: Outer capsid protein VP1

Chain i:  99%



- Molecule 11: RNA (60-MER)

Chain a2:  100%



- Molecule 11: RNA (60-MER)

Chain b2:  98%

Chain b2:  100%

U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	U15	U16	U17	U18	U19	U20	U21	U22	U23	U24	U25	U26	U27	U28	U29	U30	U31	U32	U33	U34	U35	U36	U37	U38	U39	U40	U41	U42	U43	U44	U45	U46	U47	U48	U49	U50	U51	U52	U53	U54	U55	U56	U57	U58	U59	U60
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99323	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00547	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	0/10261	0.50	0/14016
2	B	0.31	0/5734	0.52	0/7849
3	C	0.33	0/8516	0.49	0/11674
3	D	0.33	0/8985	0.49	0/12316
3	E	0.33	0/8755	0.49	0/12001
3	F	0.33	0/8985	0.49	0/12316
3	G	0.33	0/8696	0.49	0/11917
3	H	0.33	0/8922	0.49	0/12229
3	I	0.33	0/8439	0.49	0/11562
3	J	0.33	0/8919	0.49	0/12225
3	K	0.33	0/8696	0.49	0/11917
3	L	0.33	0/8985	0.49	0/12316
4	M	0.28	0/650	0.46	0/898
4	N	0.30	0/212	0.46	0/291
4	k	0.28	0/213	0.47	0/291
4	l	0.27	0/213	0.46	0/291
4	m	0.26	0/213	0.47	0/291
5	a5	0.15	0/654	0.73	0/1014
5	b5	0.10	0/654	0.67	0/1014
6	a6	0.10	0/889	0.68	0/1379
6	b6	0.17	0/889	0.74	0/1379
7	a1	0.16	0/1218	0.73	0/1890
7	b1	0.10	0/1218	0.68	0/1890
8	a3	0.16	0/936	0.73	0/1452
8	b3	0.10	0/936	0.68	0/1452
9	V	0.32	0/3234	0.47	0/4444
9	W	0.33	0/3234	0.48	0/4444
9	X	0.32	0/3234	0.47	0/4444
9	a	0.33	0/3234	0.48	0/4444
9	b	0.32	0/3234	0.47	0/4444
9	d	0.33	0/3234	0.48	0/4444
9	e	0.32	0/3234	0.47	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	g	0.32	0/3234	0.48	0/4444
9	h	0.32	0/3234	0.47	0/4444
9	n	0.33	0/3234	0.48	0/4444
10	Y	0.31	0/10233	0.51	0/14057
10	Z	0.31	0/10233	0.51	0/14057
10	c	0.31	0/10233	0.51	0/14057
10	f	0.31	0/10233	0.51	0/14057
10	i	0.31	0/10233	0.51	0/14057
11	a2	0.16	0/1406	0.74	0/2182
11	b2	0.10	0/1406	0.68	0/2182
All	All	0.31	0/199105	0.51	0/274959

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [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	A	1271/1273 (100%)	1212 (95%)	59 (5%)	0	100	100
2	B	716/718 (100%)	688 (96%)	28 (4%)	0	100	100
3	C	1073/1138 (94%)	1026 (96%)	47 (4%)	0	100	100
3	D	1136/1138 (100%)	1097 (97%)	39 (3%)	0	100	100
3	E	1104/1138 (97%)	1064 (96%)	40 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	1136/1138 (100%)	1094 (96%)	42 (4%)	0	100	100
3	G	1096/1138 (96%)	1056 (96%)	40 (4%)	0	100	100
3	H	1128/1138 (99%)	1070 (95%)	58 (5%)	0	100	100
3	I	1061/1138 (93%)	1022 (96%)	39 (4%)	0	100	100
3	J	1128/1138 (99%)	1075 (95%)	53 (5%)	0	100	100
3	K	1096/1138 (96%)	1047 (96%)	49 (4%)	0	100	100
3	L	1136/1138 (100%)	1083 (95%)	53 (5%)	0	100	100
4	M	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
4	N	28/94 (30%)	28 (100%)	0	0	100	100
4	k	28/94 (30%)	26 (93%)	2 (7%)	0	100	100
4	l	28/94 (30%)	27 (96%)	1 (4%)	0	100	100
4	m	28/94 (30%)	27 (96%)	1 (4%)	0	100	100
9	V	409/411 (100%)	401 (98%)	8 (2%)	0	100	100
9	W	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
9	X	409/411 (100%)	403 (98%)	6 (2%)	0	100	100
9	a	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
9	b	409/411 (100%)	402 (98%)	7 (2%)	0	100	100
9	d	409/411 (100%)	400 (98%)	9 (2%)	0	100	100
9	e	409/411 (100%)	403 (98%)	6 (2%)	0	100	100
9	g	409/411 (100%)	397 (97%)	12 (3%)	0	100	100
9	h	409/411 (100%)	401 (98%)	8 (2%)	0	100	100
9	n	409/411 (100%)	397 (97%)	12 (3%)	0	100	100
10	Y	1295/1297 (100%)	1254 (97%)	41 (3%)	0	100	100
10	Z	1295/1297 (100%)	1255 (97%)	40 (3%)	0	100	100
10	c	1295/1297 (100%)	1255 (97%)	40 (3%)	0	100	100
10	f	1295/1297 (100%)	1253 (97%)	42 (3%)	0	100	100
10	i	1295/1297 (100%)	1255 (97%)	39 (3%)	1 (0%)	48	77
All	All	23850/24436 (98%)	23009 (96%)	840 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	i	1291	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1092/1092 (100%)	1085 (99%)	7 (1%)	84	90
2	B	619/619 (100%)	615 (99%)	4 (1%)	84	90
3	C	917/972 (94%)	913 (100%)	4 (0%)	89	93
3	D	972/972 (100%)	967 (100%)	5 (0%)	86	91
3	E	946/972 (97%)	938 (99%)	8 (1%)	79	87
3	F	972/972 (100%)	962 (99%)	10 (1%)	73	84
3	G	938/972 (96%)	933 (100%)	5 (0%)	86	91
3	H	964/972 (99%)	954 (99%)	10 (1%)	73	84
3	I	910/972 (94%)	905 (100%)	5 (0%)	86	91
3	J	963/972 (99%)	957 (99%)	6 (1%)	84	90
3	K	938/972 (96%)	930 (99%)	8 (1%)	75	85
3	L	972/972 (100%)	963 (99%)	9 (1%)	75	85
4	M	73/73 (100%)	71 (97%)	2 (3%)	40	65
4	N	24/73 (33%)	24 (100%)	0	100	100
4	k	24/73 (33%)	24 (100%)	0	100	100
4	l	24/73 (33%)	24 (100%)	0	100	100
4	m	24/73 (33%)	24 (100%)	0	100	100
9	V	325/325 (100%)	322 (99%)	3 (1%)	75	85
9	W	325/325 (100%)	323 (99%)	2 (1%)	84	90
9	X	325/325 (100%)	322 (99%)	3 (1%)	75	85
9	a	325/325 (100%)	322 (99%)	3 (1%)	75	85
9	b	325/325 (100%)	324 (100%)	1 (0%)	91	94
9	d	325/325 (100%)	323 (99%)	2 (1%)	84	90
9	e	325/325 (100%)	323 (99%)	2 (1%)	84	90
9	g	325/325 (100%)	322 (99%)	3 (1%)	75	85
9	h	325/325 (100%)	322 (99%)	3 (1%)	75	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	n	325/325 (100%)	323 (99%)	2 (1%)	84	90
10	Y	1089/1089 (100%)	1077 (99%)	12 (1%)	70	82
10	Z	1089/1089 (100%)	1081 (99%)	8 (1%)	81	88
10	c	1089/1089 (100%)	1082 (99%)	7 (1%)	84	90
10	f	1089/1089 (100%)	1081 (99%)	8 (1%)	81	88
10	i	1089/1089 (100%)	1079 (99%)	10 (1%)	75	85
All	All	20067/20491 (98%)	19915 (99%)	152 (1%)	77	87

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	TRP
1	A	89	ASP
1	A	486	TYR
1	A	561	LEU
1	A	738	GLN
1	A	777	TYR
1	A	780	ASP
2	B	121	TYR
2	B	179	TYR
2	B	181	ASP
2	B	624	ASP
3	C	429	ASN
3	C	886	ASP
3	C	1012	ARG
3	C	1169	TRP
3	D	152	MET
3	D	206	LEU
3	D	439	THR
3	D	835	HIS
3	D	1169	TRP
3	E	125	ARG
3	E	178	HIS
3	E	209	ASN
3	E	483	VAL
3	E	829	THR
3	E	1050	ASP
3	E	1132	ARG
3	E	1203	THR
3	F	105	SER

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Mol	Chain	Res	Type
3	F	106	MET
3	F	143	ASP
3	F	232	THR
3	F	740	LYS
3	F	801	ARG
3	F	835	HIS
3	F	926	TYR
3	F	930	ARG
3	F	1012	ARG
3	G	209	ASN
3	G	552	ASP
3	G	1012	ARG
3	G	1132	ARG
3	G	1203	THR
3	H	137	ARG
3	H	150	THR
3	H	193	LEU
3	H	740	LYS
3	H	835	HIS
3	H	926	TYR
3	H	930	ARG
3	H	1012	ARG
3	H	1050	ASP
3	H	1091	GLN
3	I	316	THR
3	I	1012	ARG
3	I	1047	TYR
3	I	1203	THR
3	I	1211	ARG
3	J	232	THR
3	J	322	THR
3	J	483	VAL
3	J	617	HIS
3	J	835	HIS
3	J	958	HIS
3	K	168	ARG
3	K	518	LEU
3	K	519	GLN
3	K	1012	ARG
3	K	1047	TYR
3	K	1169	TRP
3	K	1205	ASP

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Mol	Chain	Res	Type
3	K	1211	ARG
3	L	77	ASP
3	L	123	ASN
3	L	193	LEU
3	L	257	ARG
3	L	635	GLN
3	L	801	ARG
3	L	930	ARG
3	L	981	ASN
3	L	1091	GLN
4	M	85	ASP
4	M	94	THR
9	V	35	ARG
9	V	158	HIS
9	V	255	ARG
9	W	11	TYR
9	W	255	ARG
9	X	35	ARG
9	X	44	LEU
9	X	255	ARG
10	Y	71	HIS
10	Y	243	GLN
10	Y	711	ASP
10	Y	929	MET
10	Y	932	GLN
10	Y	955	VAL
10	Y	963	ARG
10	Y	1204	LEU
10	Y	1209	ASP
10	Y	1225	ASP
10	Y	1283	GLN
10	Y	1296	TYR
10	Z	164	VAL
10	Z	243	GLN
10	Z	410	THR
10	Z	439	SER
10	Z	676	ARG
10	Z	711	ASP
10	Z	929	MET
10	Z	1296	TYR
9	a	11	TYR
9	a	252	ASP

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Mol	Chain	Res	Type
9	a	255	ARG
9	b	255	ARG
10	c	243	GLN
10	c	658	VAL
10	c	711	ASP
10	c	929	MET
10	c	1205	LEU
10	c	1283	GLN
10	c	1296	TYR
9	d	11	TYR
9	d	255	ARG
9	e	245	GLN
9	e	255	ARG
10	f	71	HIS
10	f	243	GLN
10	f	610	THR
10	f	711	ASP
10	f	929	MET
10	f	1225	ASP
10	f	1283	GLN
10	f	1296	TYR
9	g	11	TYR
9	g	38	THR
9	g	255	ARG
9	h	158	HIS
9	h	195	GLN
9	h	255	ARG
10	i	71	HIS
10	i	197	HIS
10	i	243	GLN
10	i	309	ASN
10	i	711	ASP
10	i	929	MET
10	i	1225	ASP
10	i	1261	THR
10	i	1283	GLN
10	i	1296	TYR
9	n	11	TYR
9	n	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1206	HIS
3	D	209	ASN
3	F	104	GLN
3	F	523	ASN
3	F	906	ASN
3	G	748	GLN
3	I	287	GLN
3	J	353	GLN
3	J	580	HIS
3	J	962	GLN
3	K	748	GLN
3	L	135	HIS
3	L	140	HIS
3	L	1091	GLN
9	X	273	HIS
10	Y	630	GLN
10	Z	685	ASN
9	a	338	HIS
9	b	158	HIS
10	f	630	GLN
9	g	158	HIS
10	i	309	ASN
10	i	1151	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	a2	59/60 (98%)	0	0
11	b2	59/60 (98%)	0	0
5	a5	27/28 (96%)	0	0
5	b5	27/28 (96%)	0	0
6	a6	37/38 (97%)	0	0
6	b6	37/38 (97%)	0	0
7	a1	51/52 (98%)	0	0
7	b1	51/52 (98%)	0	0
8	a3	39/40 (97%)	0	0
8	b3	39/40 (97%)	0	0
All	All	426/436 (97%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

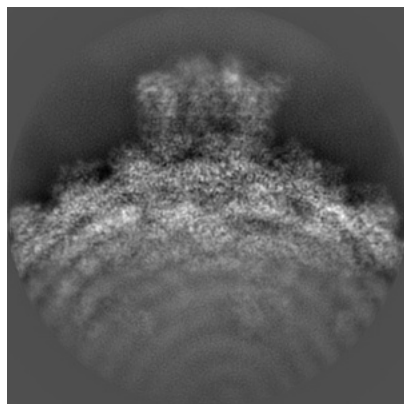
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29244. These allow visual inspection of the internal detail of the map and identification of artifacts.

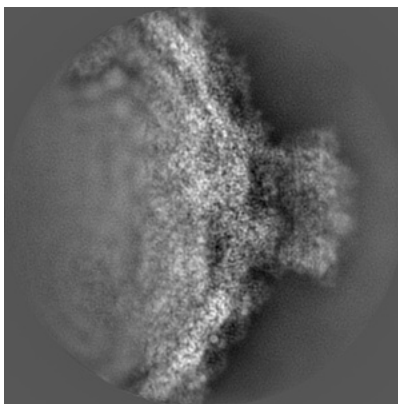
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

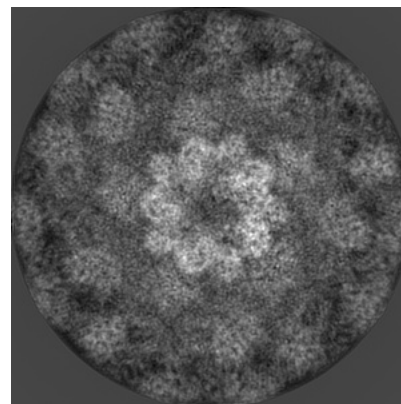
#### 6.1.1 Primary map



X

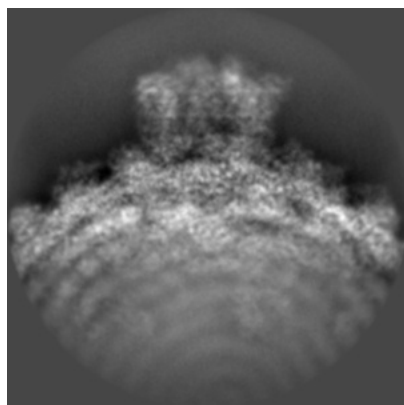


Y

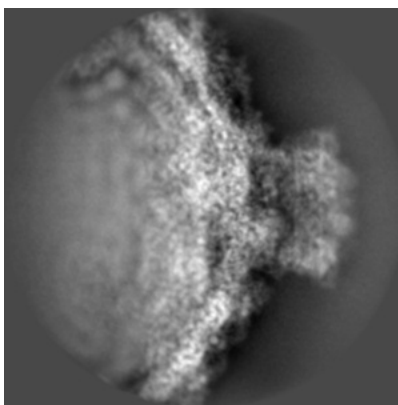


Z

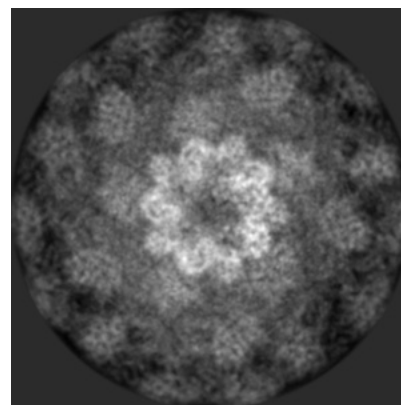
#### 6.1.2 Raw map



X



Y

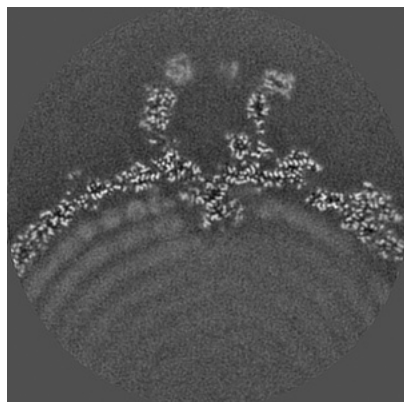


Z

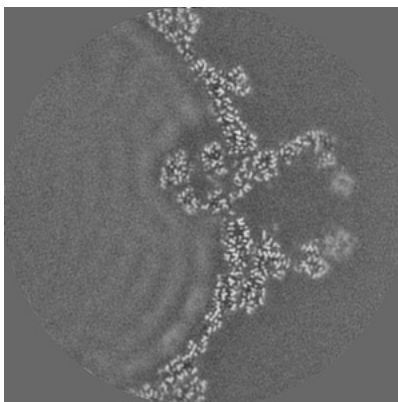
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

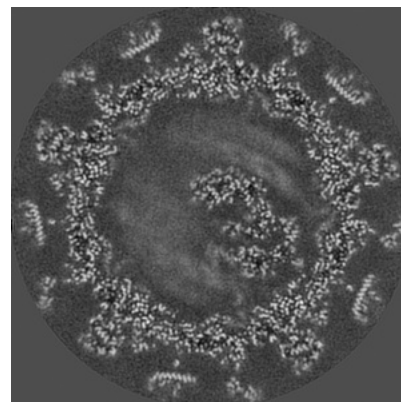
### 6.2.1 Primary map



X Index: 160

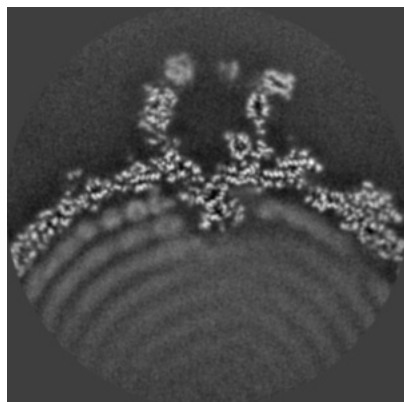


Y Index: 160

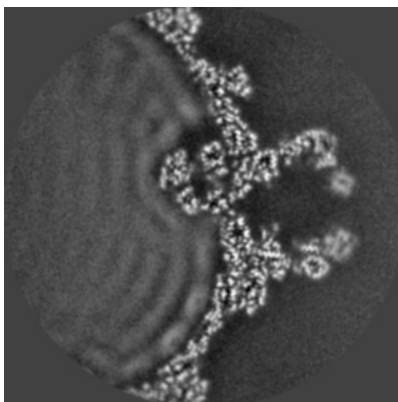


Z Index: 160

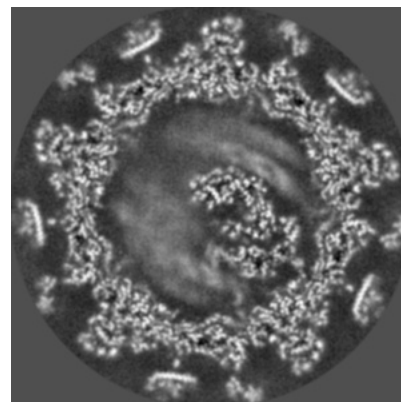
### 6.2.2 Raw map



X Index: 160



Y Index: 160

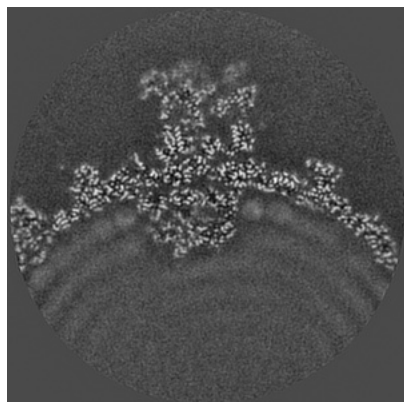


Z Index: 160

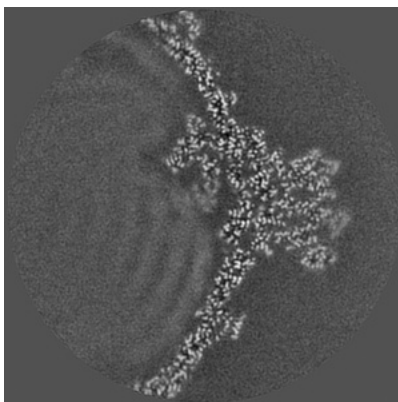
The images above show central slices of the map in three orthogonal directions.

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

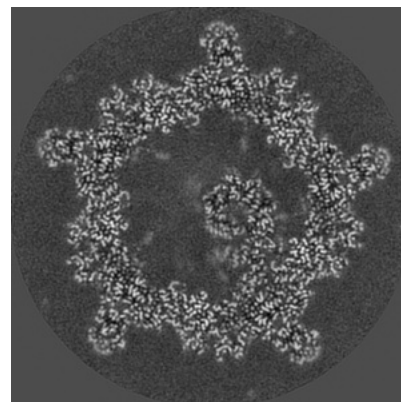
### 6.3.1 Primary map



X Index: 192

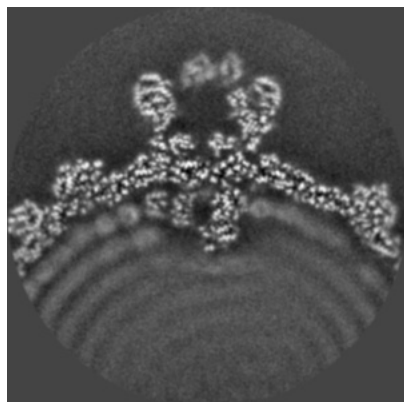


Y Index: 125

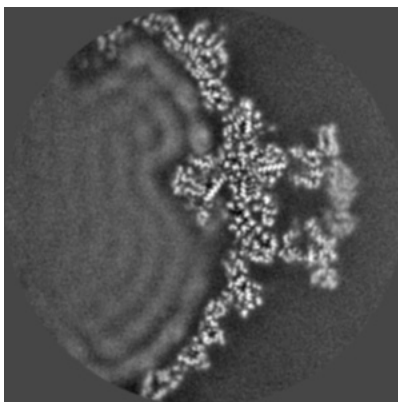


Z Index: 168

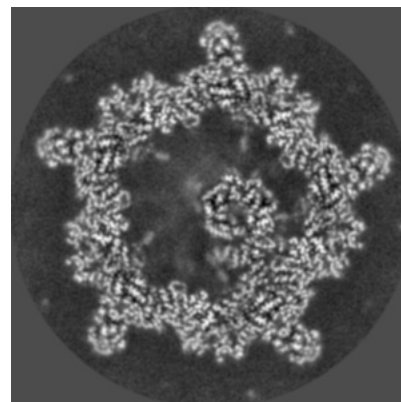
### 6.3.2 Raw map



X Index: 178



Y Index: 182



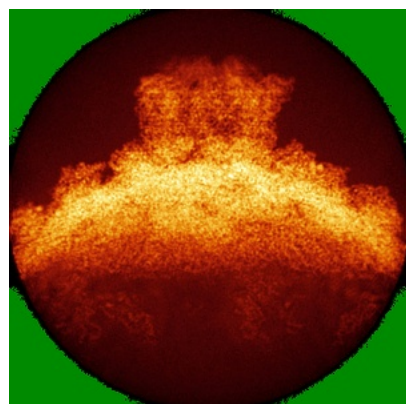
Z Index: 168

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

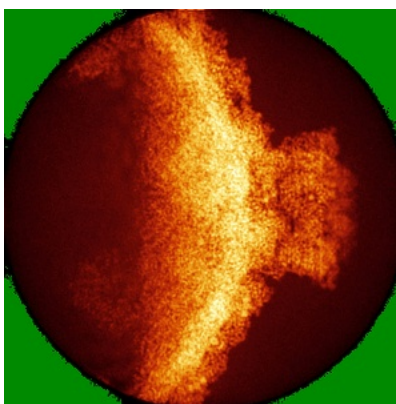


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

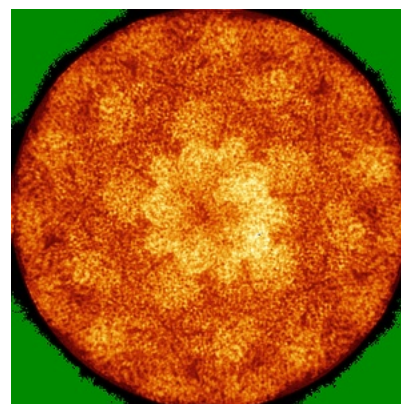
### 6.4.1 Primary map



X

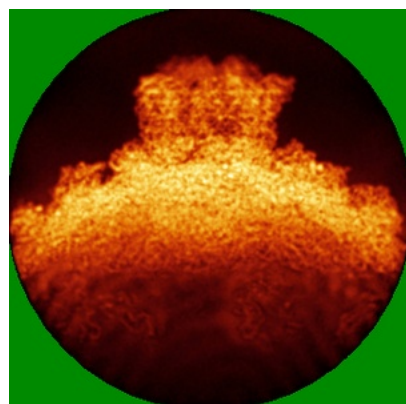


Y

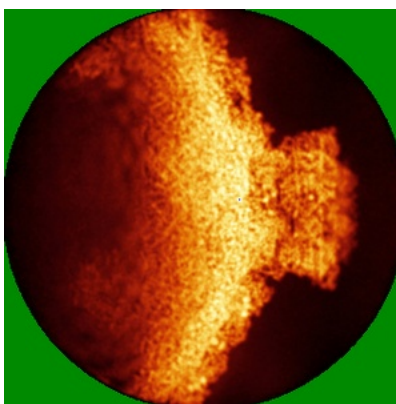


Z

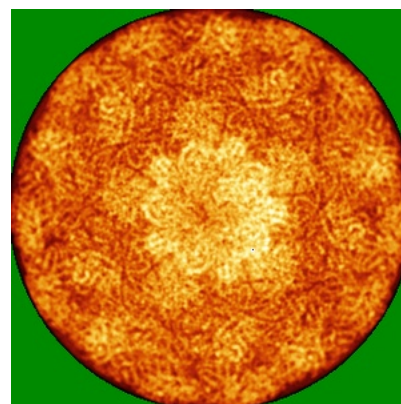
### 6.4.2 Raw map



X



Y

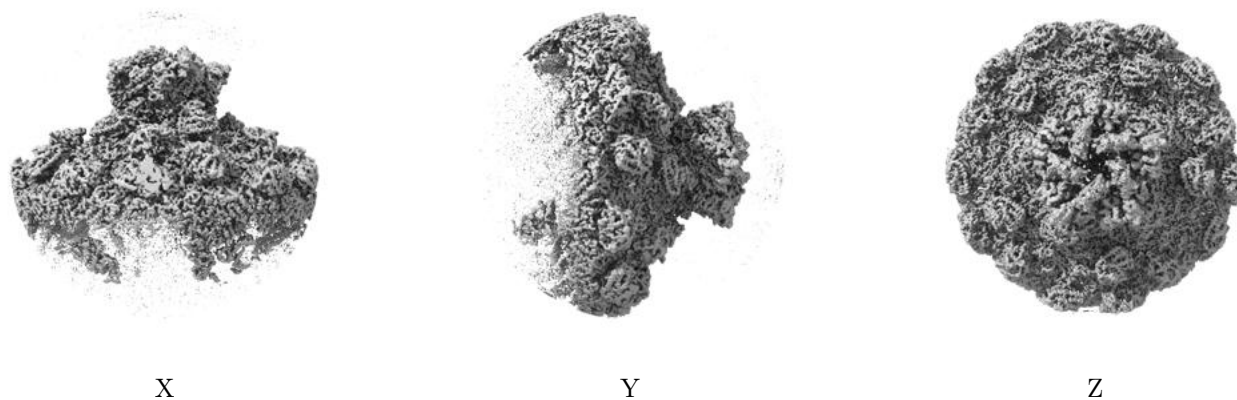


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00547. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

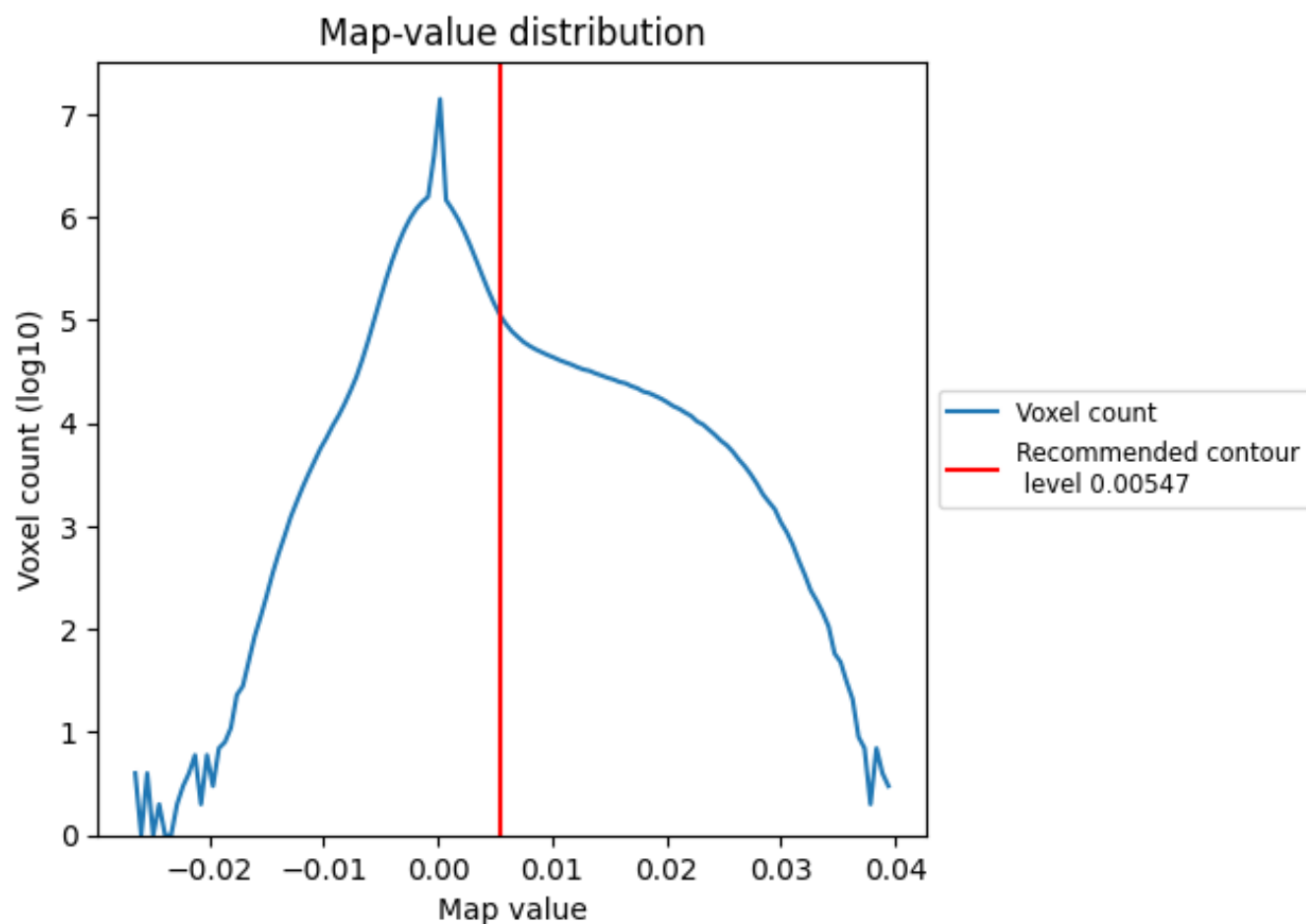
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

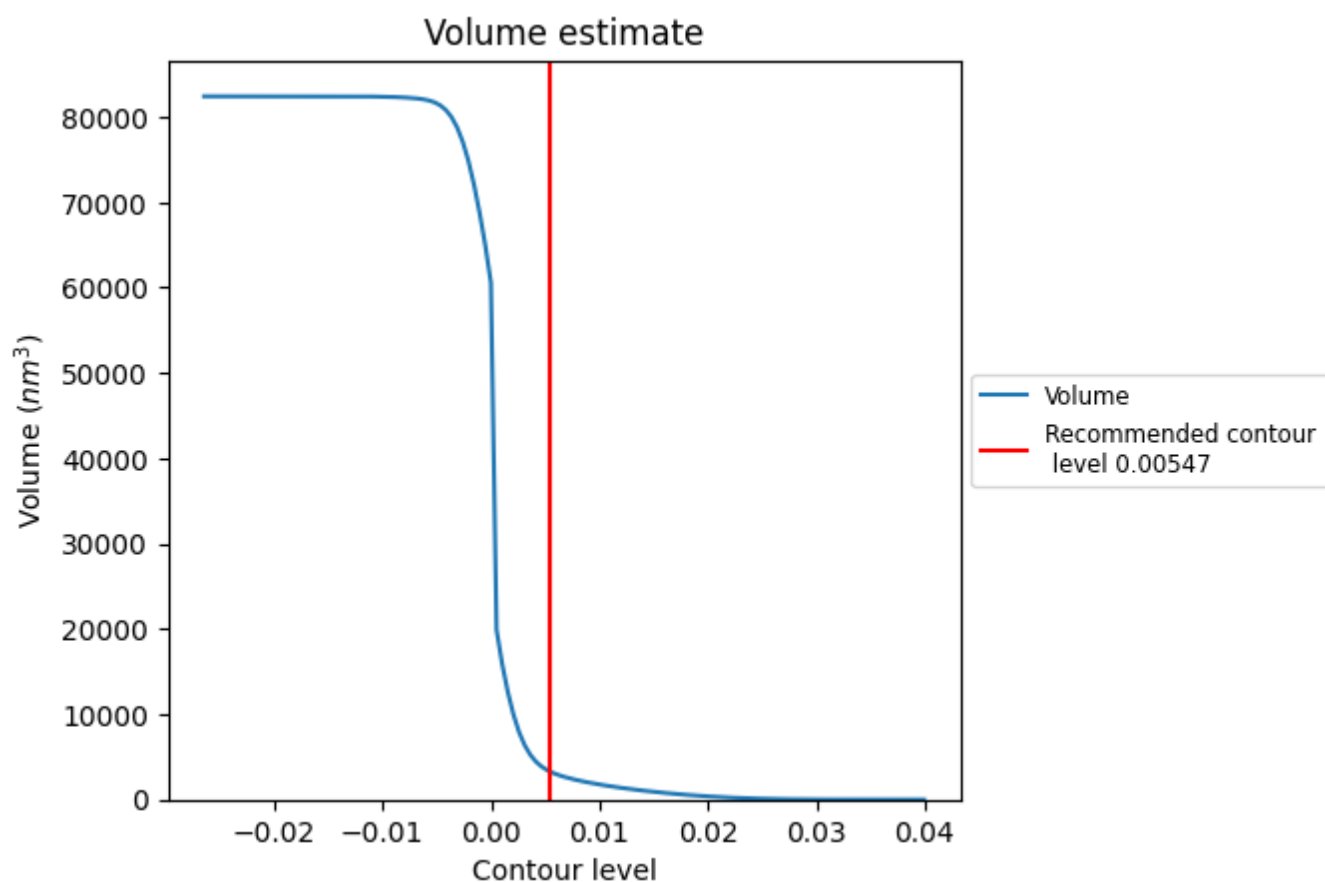
This section contains the results of statistical analysis of the map.

### 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.

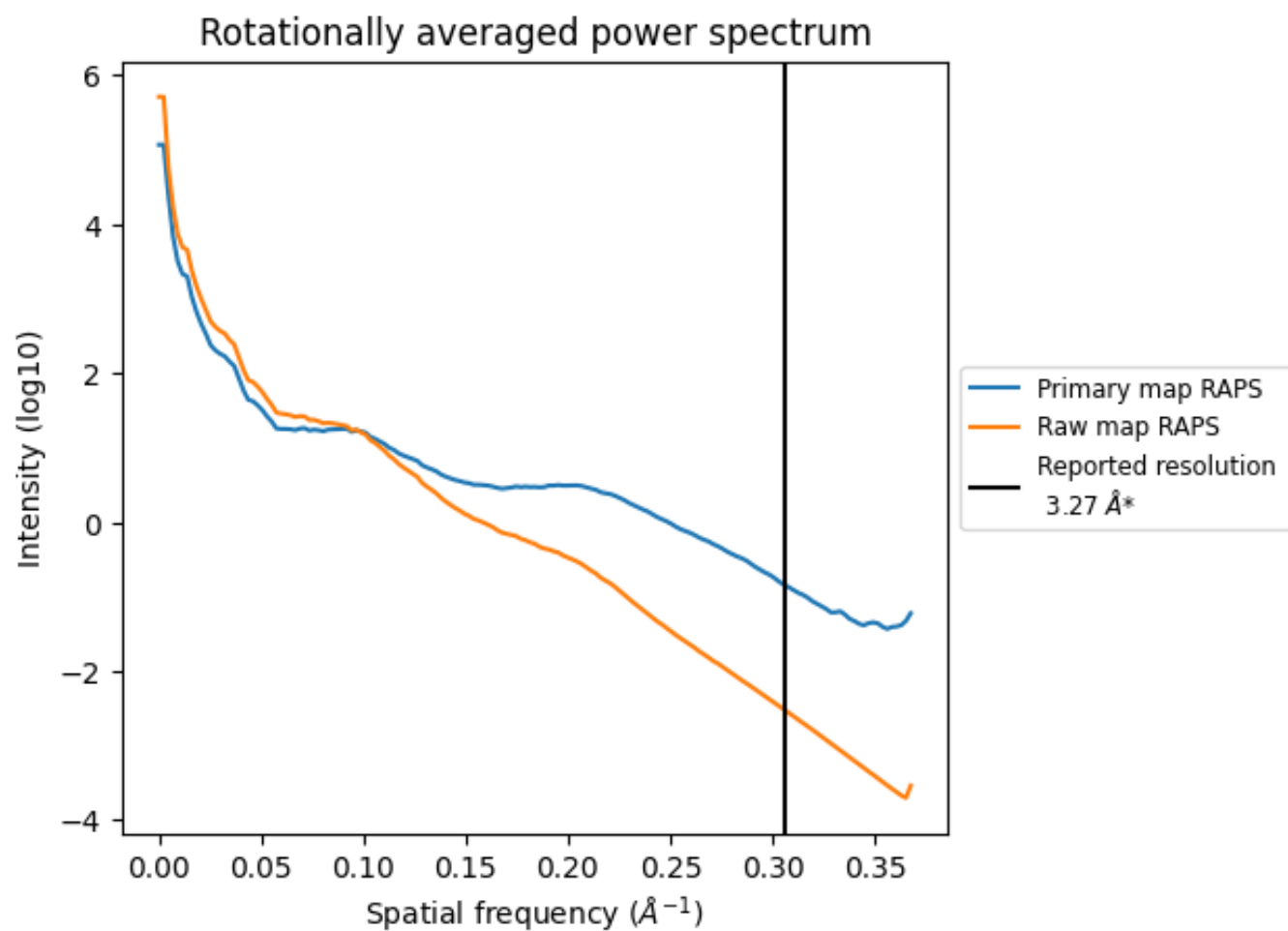
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3273  $\text{nm}^3$ ; this corresponds to an approximate mass of 2956 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 ⓘ

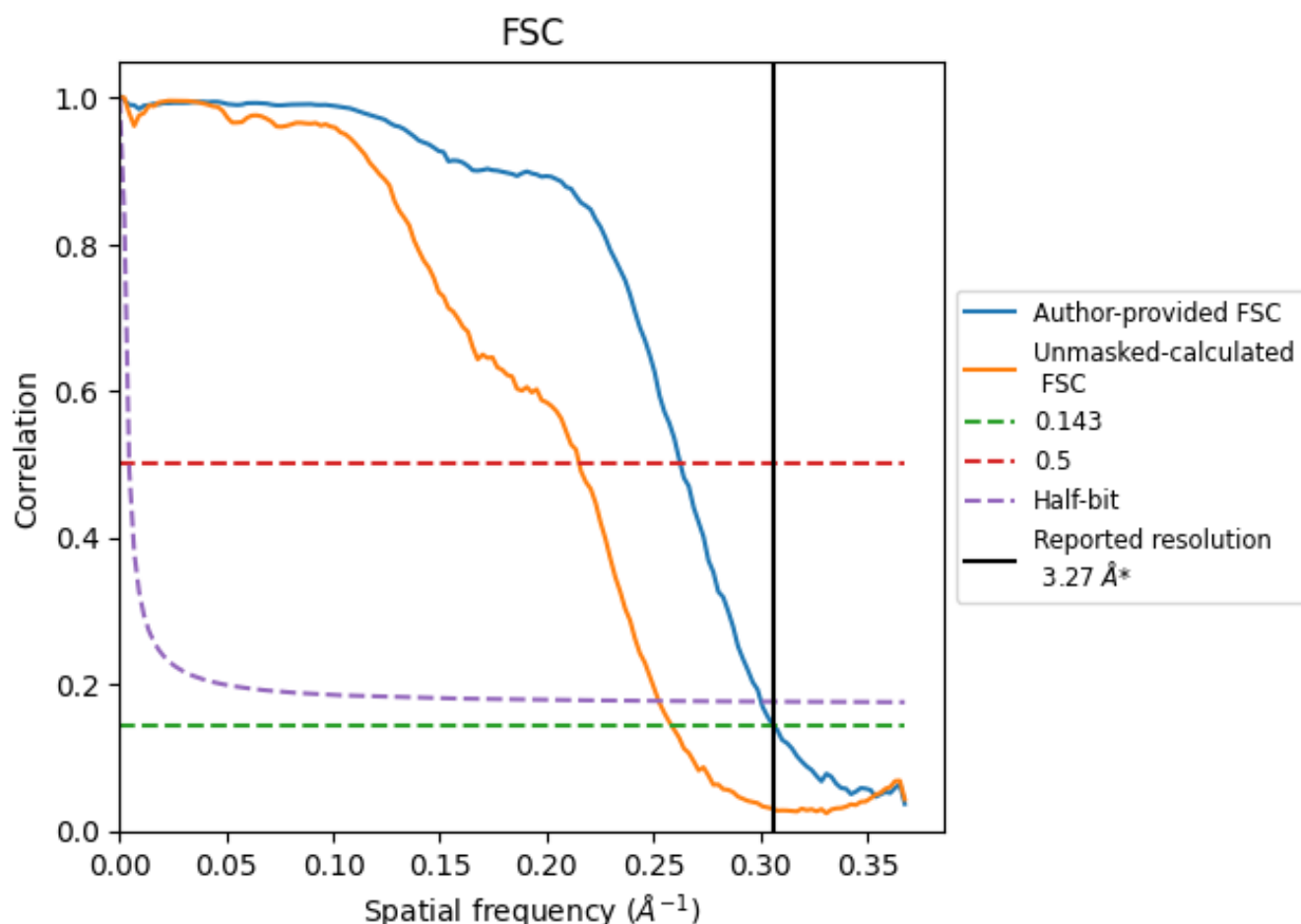


\*Reported resolution corresponds to spatial frequency of 0.306  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.306 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

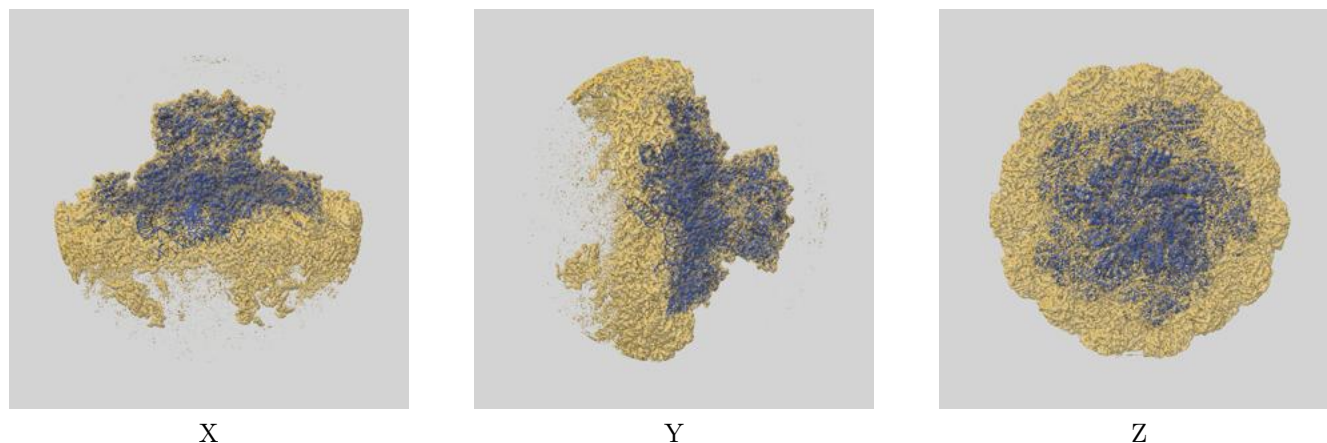
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	3.27	3.81	3.33
Unmasked-calculated*	3.87	4.65	3.96

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.27 by more than 10 %

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

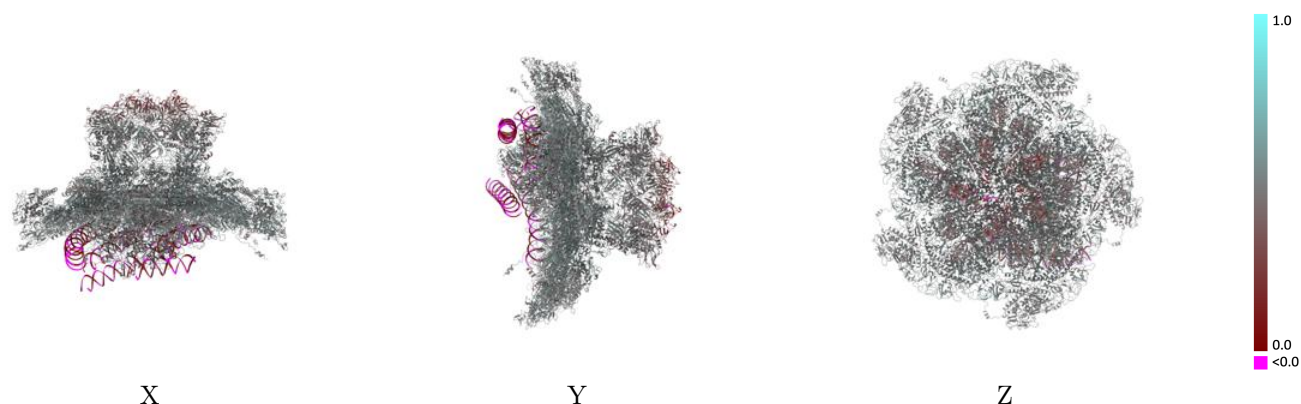
This section contains information regarding the fit between EMDB map EMD-29244 and PDB model 8FJL. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



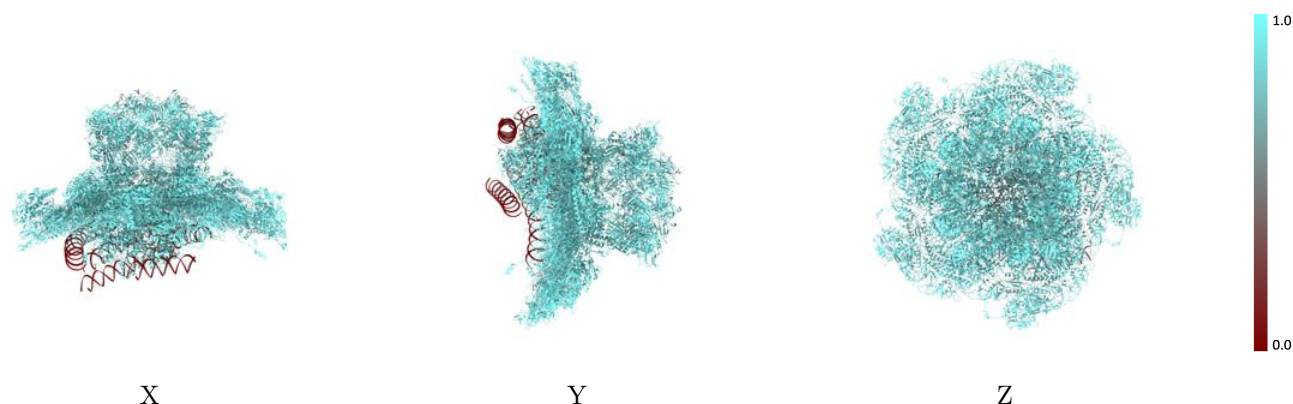
The images above show the 3D surface view of the map at the recommended contour level 0.00547 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



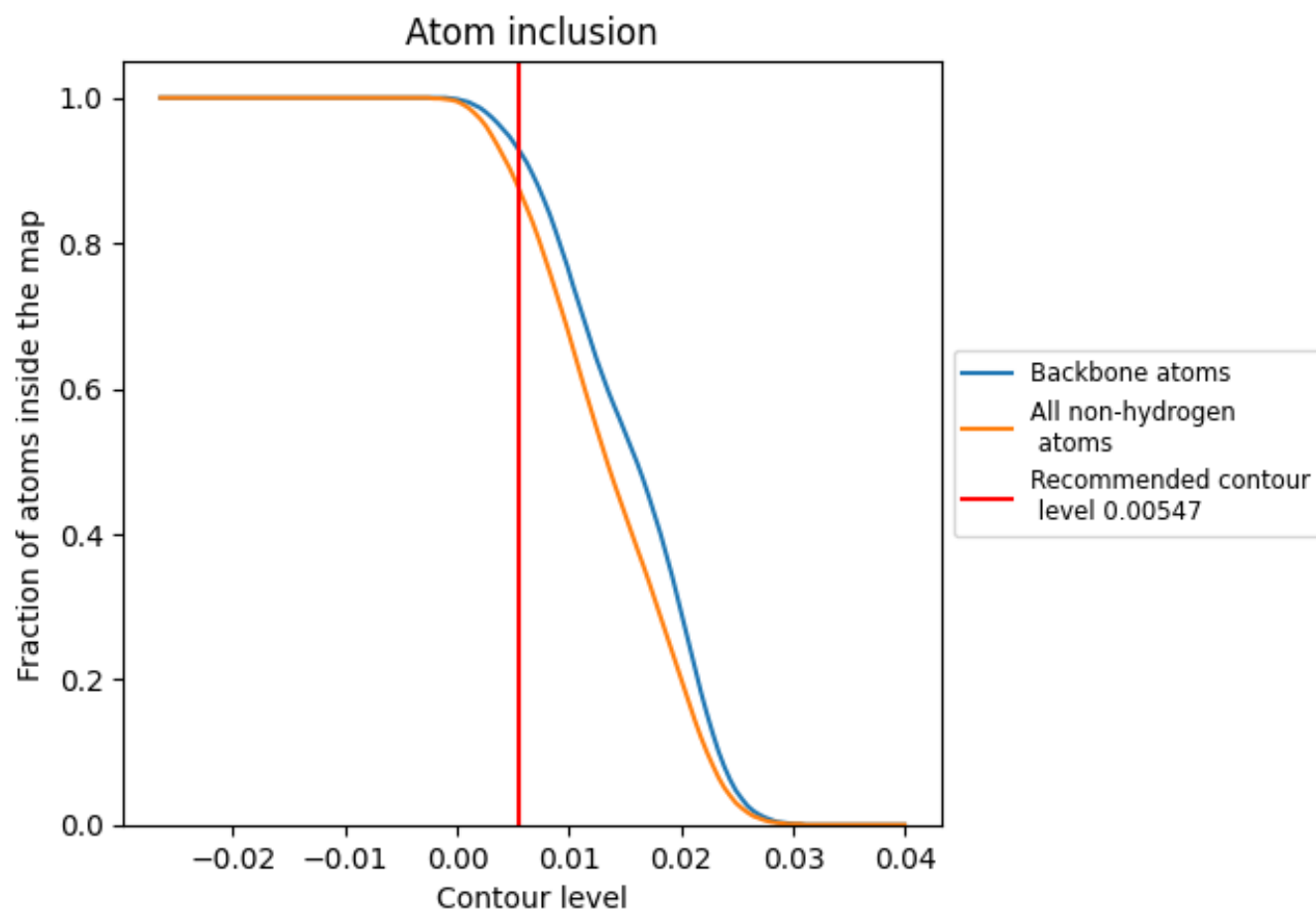
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00547).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.00547) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.4650
A	 0.8520	 0.4790
B	 0.8040	 0.4440
C	 0.9020	 0.5120
D	 0.8940	 0.4960
E	 0.9030	 0.5020
F	 0.9010	 0.4910
G	 0.9130	 0.5110
H	 0.9070	 0.5030
I	 0.9100	 0.5130
J	 0.9060	 0.4970
K	 0.9080	 0.5090
L	 0.9010	 0.5000
M	 0.8530	 0.4860
N	 0.8370	 0.4960
V	 0.9300	 0.4800
W	 0.9430	 0.4970
X	 0.9300	 0.4870
Y	 0.9160	 0.4530
Z	 0.9140	 0.4540
a	 0.9410	 0.5080
a1	 0.3430	 0.0910
a2	 0.0760	 0.0290
a3	 0.0130	 0.0210
a5	 0.0580	 0.0420
a6	 0.4790	 0.0900
b	 0.9270	 0.4770
b1	 0.3560	 0.0620
b2	 0.0960	 0.0580
b3	 0.0260	 0.0230
b5	 0.0730	 0.0160
b6	 0.2970	 0.0380
c	 0.9150	 0.4550
d	 0.9460	 0.5080
e	 0.9410	 0.4880



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Chain	Atom inclusion	Q-score
f	 0.9120	 0.4560
g	 0.9430	 0.5090
h	 0.9370	 0.4950
i	 0.9190	 0.4550
k	 0.8610	 0.5080
l	 0.8420	 0.4950
m	 0.8280	 0.4750
n	 0.9500	 0.5140