wwPDB EM Validation Summary Report

Jan 1, 2025 – 03:42 PM EST

PDB ID	:	8W9Q
EMDB ID	:	EMD-37379
Title	:	Structure of partial Banna virus
Authors	:	Li, Z.; Cao, S.
Deposited on	:	2023-09-05
Resolution	:	5.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

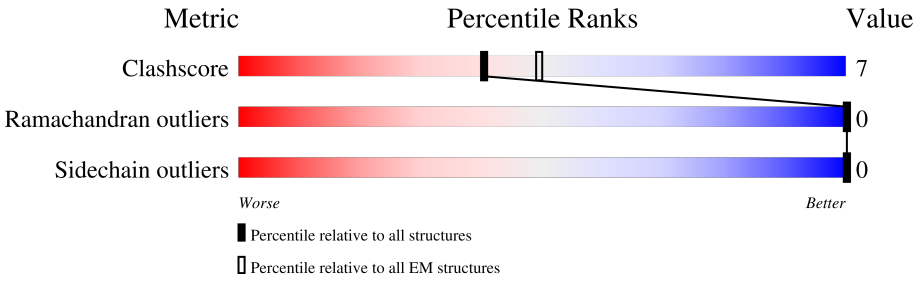
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	A	955	70% 8% 21%
1	B	955	85% 10% 6%
2	C	302	87% 12%
2	D	302	86% 12%
2	E	302	83% 15%
2	F	302	93% 6%
2	G	302	84% 14%
2	H	302	89% 10%

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Mol	Chain	Length	Quality of chain
2	I	302	88% 11%
2	J	302	89% 10%
2	K	302	90% 9%
2	L	302	86% 13%
2	M	302	86% 12%
2	N	302	84% 15%
2	O	302	88% 11%
3	P	249	82% 18%
3	Q	249	80% 19%
4	R	628	76% 19%
4	S	628	80% 19%
4	T	628	79% 20%
5	r	283	5% 95%
5	s	283	5% 95%
5	t	283	5% 95%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 61697 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 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	751	Total	C	N	O	S	0	0
			6045	3848	1025	1145	27		
1	B	902	Total	C	N	O	S	0	0
			7210	4578	1221	1384	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	LYS	ARG	conflict	UNP Q9INH3
B	97	LYS	ARG	conflict	UNP Q9INH3

- Molecule 2 is a protein called VP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	299	Total	C	N	O	S	0	0
			2288	1449	397	435	7		
2	D	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	E	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	F	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	G	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	H	299	Total	C	N	O	S	0	0
			2288	1449	397	435	7		
2	I	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	J	299	Total	C	N	O	S	0	0
			2288	1449	397	435	7		
2	K	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	L	297	Total	C	N	O	S	0	0
			2270	1438	392	433	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	N	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	O	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	136	ARG	GLN	conflict	UNP W0G587
C	185	LEU	MET	conflict	UNP W0G587
C	266	SER	ALA	conflict	UNP W0G587
D	136	ARG	GLN	conflict	UNP W0G587
D	185	LEU	MET	conflict	UNP W0G587
D	266	SER	ALA	conflict	UNP W0G587
E	136	ARG	GLN	conflict	UNP W0G587
E	185	LEU	MET	conflict	UNP W0G587
E	266	SER	ALA	conflict	UNP W0G587
F	136	ARG	GLN	conflict	UNP W0G587
F	185	LEU	MET	conflict	UNP W0G587
F	266	SER	ALA	conflict	UNP W0G587
G	136	ARG	GLN	conflict	UNP W0G587
G	185	LEU	MET	conflict	UNP W0G587
G	266	SER	ALA	conflict	UNP W0G587
H	136	ARG	GLN	conflict	UNP W0G587
H	185	LEU	MET	conflict	UNP W0G587
H	266	SER	ALA	conflict	UNP W0G587
I	136	ARG	GLN	conflict	UNP W0G587
I	185	LEU	MET	conflict	UNP W0G587
I	266	SER	ALA	conflict	UNP W0G587
J	136	ARG	GLN	conflict	UNP W0G587
J	185	LEU	MET	conflict	UNP W0G587
J	266	SER	ALA	conflict	UNP W0G587
K	136	ARG	GLN	conflict	UNP W0G587
K	185	LEU	MET	conflict	UNP W0G587
K	266	SER	ALA	conflict	UNP W0G587
L	136	ARG	GLN	conflict	UNP W0G587
L	185	LEU	MET	conflict	UNP W0G587
L	266	SER	ALA	conflict	UNP W0G587
M	136	ARG	GLN	conflict	UNP W0G587
M	185	LEU	MET	conflict	UNP W0G587

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Chain	Residue	Modelled	Actual	Comment	Reference
M	266	SER	ALA	conflict	UNP W0G587
N	136	ARG	GLN	conflict	UNP W0G587
N	185	LEU	MET	conflict	UNP W0G587
N	266	SER	ALA	conflict	UNP W0G587
O	136	ARG	GLN	conflict	UNP W0G587
O	185	LEU	MET	conflict	UNP W0G587
O	266	SER	ALA	conflict	UNP W0G587

- Molecule 3 is a protein called VP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	249	Total	C	N	O	S	0	0
			2014	1276	353	377	8		
3	Q	246	Total	C	N	O	S	0	0
			1986	1258	347	373	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	79	VAL	ILE	conflict	UNP A0A2H4QDD3
Q	79	VAL	ILE	conflict	UNP A0A2H4QDD3

- Molecule 4 is a protein called VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	601	Total	C	N	O	S	0	0
			4706	2969	814	907	16		
4	S	622	Total	C	N	O	S	0	0
			4858	3060	841	941	16		
4	T	627	Total	C	N	O	S	0	0
			4900	3088	848	948	16		

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	15	ASN	SER	conflict	UNP B4Y048
R	61	LEU	ILE	conflict	UNP B4Y048
R	62	ASN	ILE	conflict	UNP B4Y048
R	65	ALA	THR	conflict	UNP B4Y048
R	80	ASN	LYS	conflict	UNP B4Y048
R	94	ILE	VAL	conflict	UNP B4Y048
R	130	VAL	ILE	conflict	UNP B4Y048

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Chain	Residue	Modelled	Actual	Comment	Reference
R	154	VAL	ILE	conflict	UNP B4Y048
R	235	ALA	SER	conflict	UNP B4Y048
R	271	VAL	THR	conflict	UNP B4Y048
R	278	ILE	VAL	conflict	UNP B4Y048
R	307	LEU	MET	conflict	UNP B4Y048
R	322	ASN	THR	conflict	UNP B4Y048
R	369	ALA	VAL	conflict	UNP B4Y048
R	436	ASP	GLU	conflict	UNP B4Y048
R	439	GLN	LYS	conflict	UNP B4Y048
R	444	THR	ALA	conflict	UNP B4Y048
R	470	LYS	ARG	conflict	UNP B4Y048
R	500	THR	ALA	conflict	UNP B4Y048
R	524	VAL	ILE	conflict	UNP B4Y048
R	537	ASN	ASP	conflict	UNP B4Y048
R	539	SER	ASP	conflict	UNP B4Y048
R	543	SER	LEU	conflict	UNP B4Y048
R	545	ASN	LYS	conflict	UNP B4Y048
R	547	ARG	LYS	conflict	UNP B4Y048
R	575	ALA	THR	conflict	UNP B4Y048
R	628	PRO	SER	conflict	UNP B4Y048
S	15	ASN	SER	conflict	UNP B4Y048
S	61	LEU	ILE	conflict	UNP B4Y048
S	62	ASN	ILE	conflict	UNP B4Y048
S	65	ALA	THR	conflict	UNP B4Y048
S	80	ASN	LYS	conflict	UNP B4Y048
S	94	ILE	VAL	conflict	UNP B4Y048
S	130	VAL	ILE	conflict	UNP B4Y048
S	154	VAL	ILE	conflict	UNP B4Y048
S	235	ALA	SER	conflict	UNP B4Y048
S	271	VAL	THR	conflict	UNP B4Y048
S	278	ILE	VAL	conflict	UNP B4Y048
S	307	LEU	MET	conflict	UNP B4Y048
S	322	ASN	THR	conflict	UNP B4Y048
S	369	ALA	VAL	conflict	UNP B4Y048
S	436	ASP	GLU	conflict	UNP B4Y048
S	439	GLN	LYS	conflict	UNP B4Y048
S	444	THR	ALA	conflict	UNP B4Y048
S	470	LYS	ARG	conflict	UNP B4Y048
S	500	THR	ALA	conflict	UNP B4Y048
S	524	VAL	ILE	conflict	UNP B4Y048
S	537	ASN	ASP	conflict	UNP B4Y048
S	539	SER	ASP	conflict	UNP B4Y048

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Chain	Residue	Modelled	Actual	Comment	Reference
S	543	SER	LEU	conflict	UNP B4Y048
S	545	ASN	LYS	conflict	UNP B4Y048
S	547	ARG	LYS	conflict	UNP B4Y048
S	575	ALA	THR	conflict	UNP B4Y048
S	628	PRO	SER	conflict	UNP B4Y048
T	15	ASN	SER	conflict	UNP B4Y048
T	61	LEU	ILE	conflict	UNP B4Y048
T	62	ASN	ILE	conflict	UNP B4Y048
T	65	ALA	THR	conflict	UNP B4Y048
T	80	ASN	LYS	conflict	UNP B4Y048
T	94	ILE	VAL	conflict	UNP B4Y048
T	130	VAL	ILE	conflict	UNP B4Y048
T	154	VAL	ILE	conflict	UNP B4Y048
T	235	ALA	SER	conflict	UNP B4Y048
T	271	VAL	THR	conflict	UNP B4Y048
T	278	ILE	VAL	conflict	UNP B4Y048
T	307	LEU	MET	conflict	UNP B4Y048
T	322	ASN	THR	conflict	UNP B4Y048
T	369	ALA	VAL	conflict	UNP B4Y048
T	436	ASP	GLU	conflict	UNP B4Y048
T	439	GLN	LYS	conflict	UNP B4Y048
T	444	THR	ALA	conflict	UNP B4Y048
T	470	LYS	ARG	conflict	UNP B4Y048
T	500	THR	ALA	conflict	UNP B4Y048
T	524	VAL	ILE	conflict	UNP B4Y048
T	537	ASN	ASP	conflict	UNP B4Y048
T	539	SER	ASP	conflict	UNP B4Y048
T	543	SER	LEU	conflict	UNP B4Y048
T	545	ASN	LYS	conflict	UNP B4Y048
T	547	ARG	LYS	conflict	UNP B4Y048
T	575	ALA	THR	conflict	UNP B4Y048
T	628	PRO	SER	conflict	UNP B4Y048

- Molecule 5 is a protein called VP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	r	15	Total	C	N	O	0	0
			117	73	20	24		
5	s	15	Total	C	N	O	0	0
			117	73	20	24		
5	t	15	Total	C	N	O	0	0
			117	73	20	24		

There are 12 discrepancies between the modelled and reference sequences:

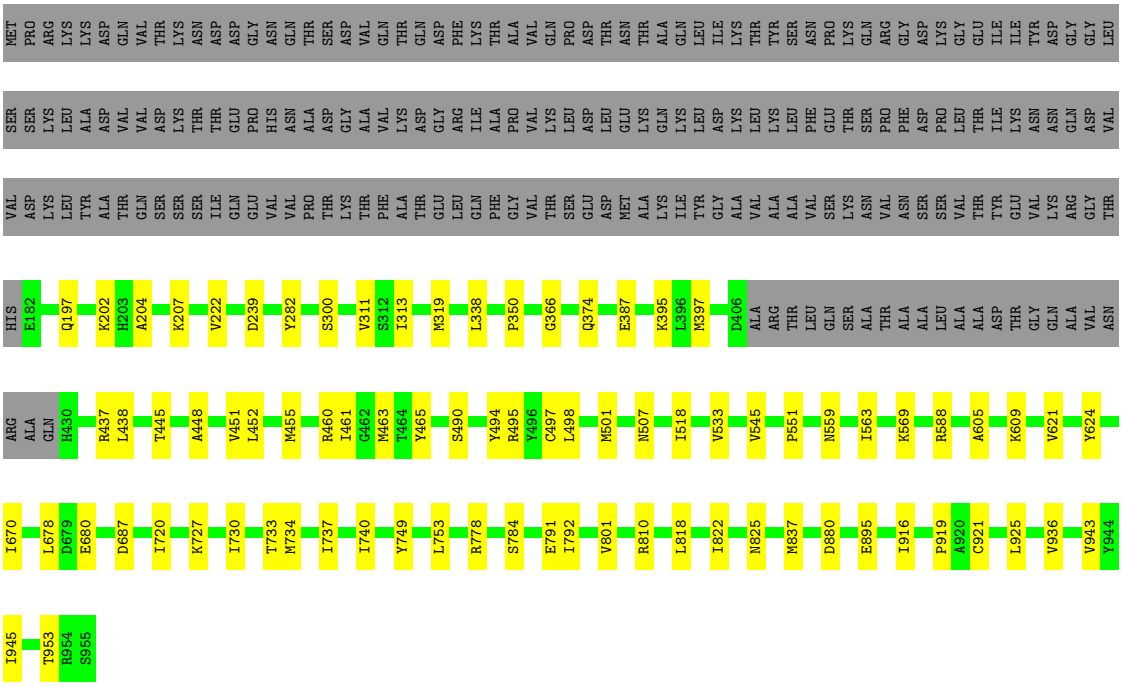
Chain	Residue	Modelled	Actual	Comment	Reference
r	150	TYR	HIS	conflict	UNP Q9YWN5
r	156	LEU	GLN	conflict	UNP Q9YWN5
r	184	THR	ALA	conflict	UNP Q9YWN5
r	191	ASN	ASP	conflict	UNP Q9YWN5
s	150	TYR	HIS	conflict	UNP Q9YWN5
s	156	LEU	GLN	conflict	UNP Q9YWN5
s	184	THR	ALA	conflict	UNP Q9YWN5
s	191	ASN	ASP	conflict	UNP Q9YWN5
t	150	TYR	HIS	conflict	UNP Q9YWN5
t	156	LEU	GLN	conflict	UNP Q9YWN5
t	184	THR	ALA	conflict	UNP Q9YWN5
t	191	ASN	ASP	conflict	UNP Q9YWN5

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.

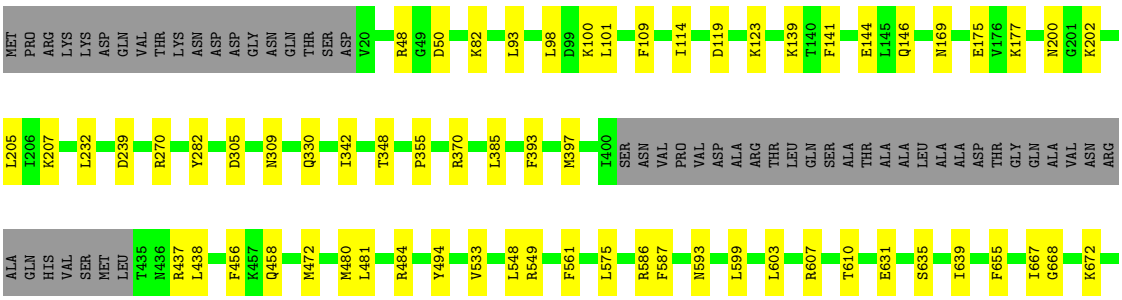
- Molecule 1: VP2

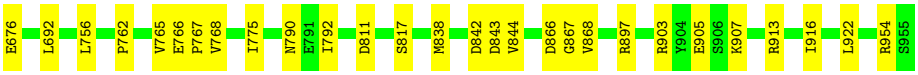
Chain A:



- Molecule 1: VP2

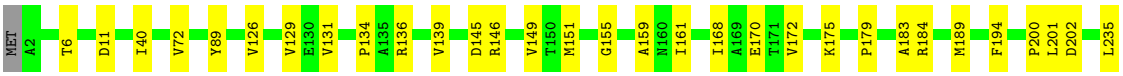
Chain B:





• Molecule 2: VP8

Chain C:

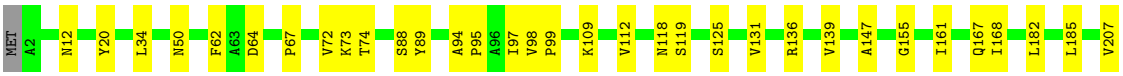


• Molecule 2: VP8

Chain D:

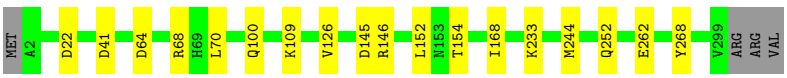
• Molecule 2: VP8

Chain E:



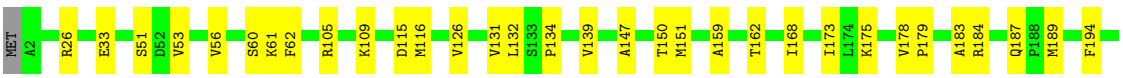
• Molecule 2: VP8

Chain F:



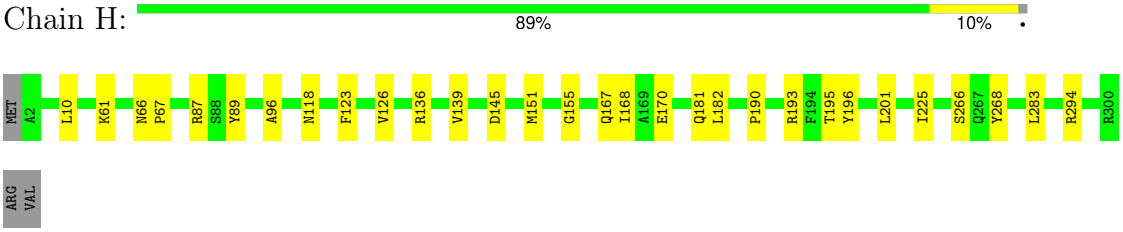
• Molecule 2: VP8

Chain G:



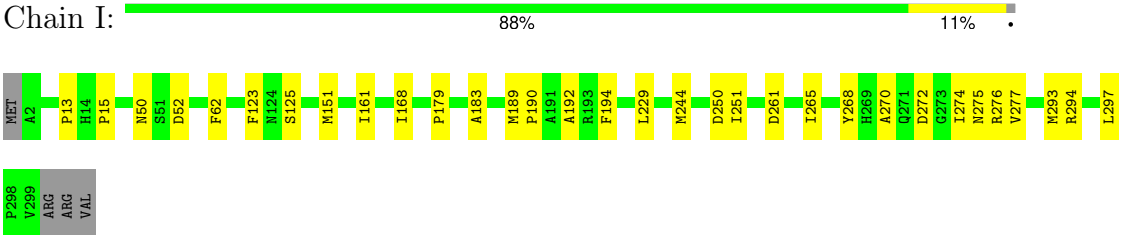
• Molecule 2: VP8

Chain H:



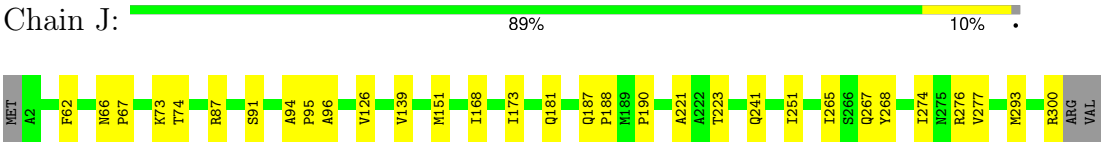
• Molecule 2: VP8

Chain I:



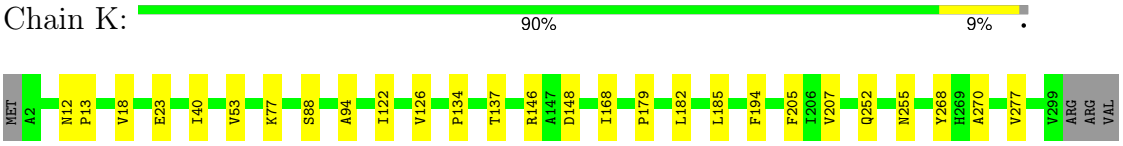
• Molecule 2: VP8

Chain J:



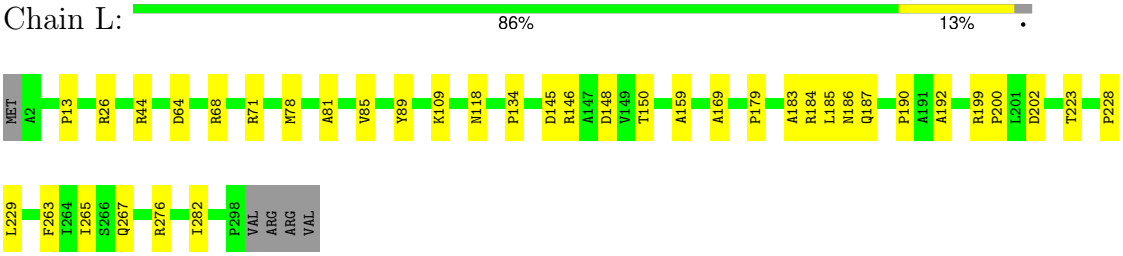
• Molecule 2: VP8

Chain K:



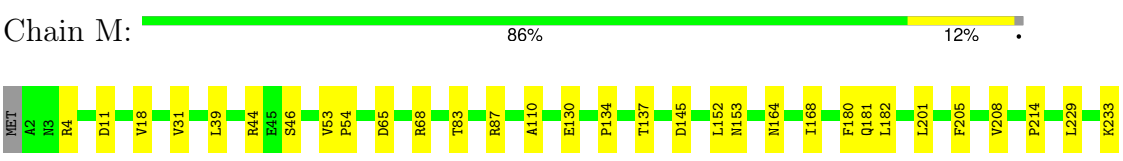
• Molecule 2: VP8

Chain L:



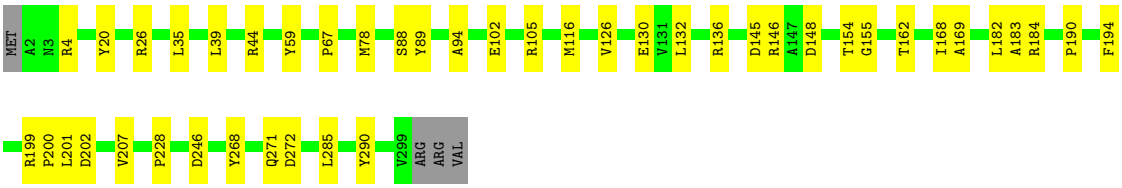
• Molecule 2: VP8

Chain M:



• Molecule 2: VP8

Chain N:

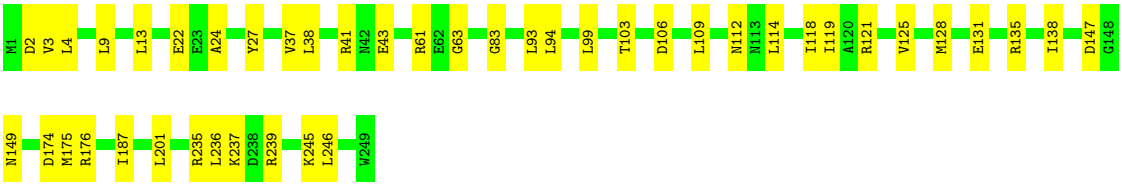


• Molecule 2: VP8

Chain O:

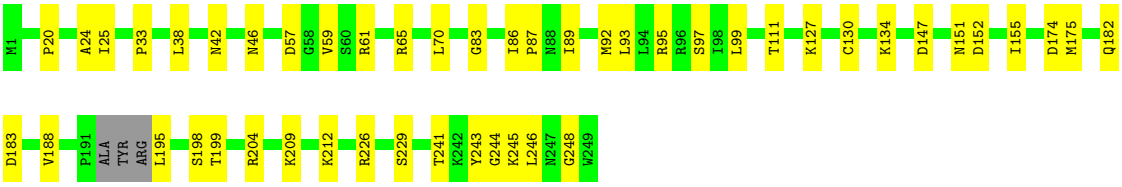
• Molecule 3: VP10

Chain P:



• Molecule 3: VP10

Chain Q:

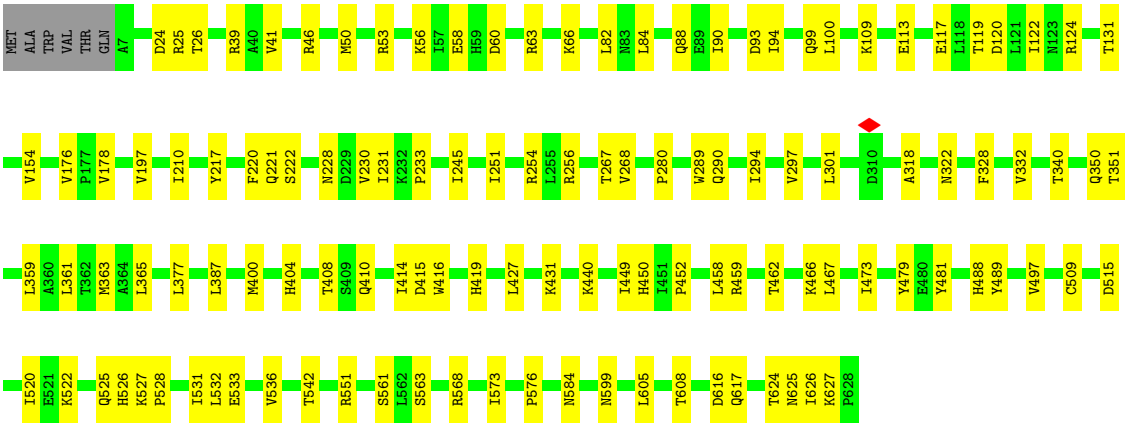


• Molecule 4: VP4

Chain R:

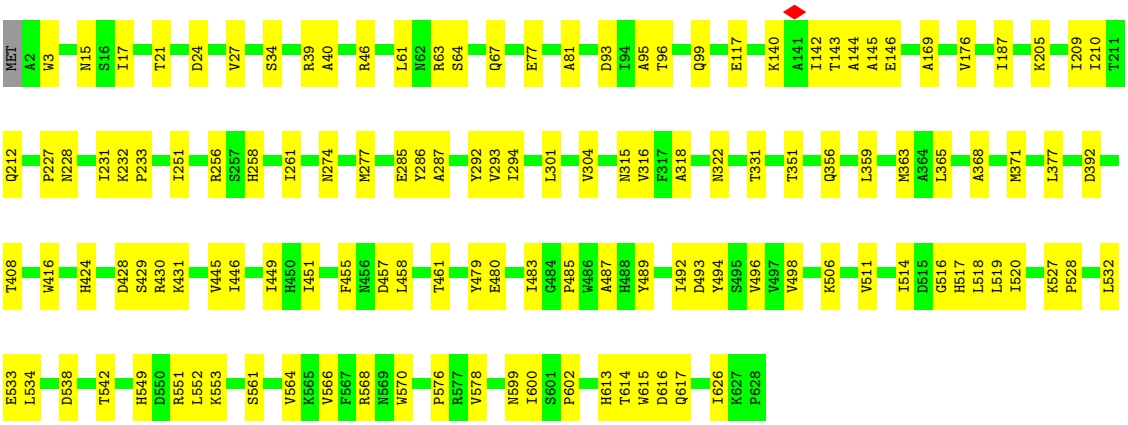
• Molecule 4: VP4

Chain S:



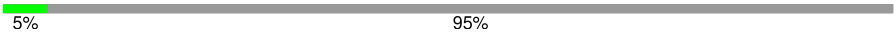
• Molecule 4: VP4

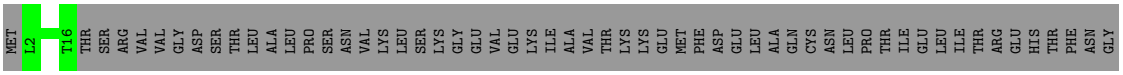
Chain T:

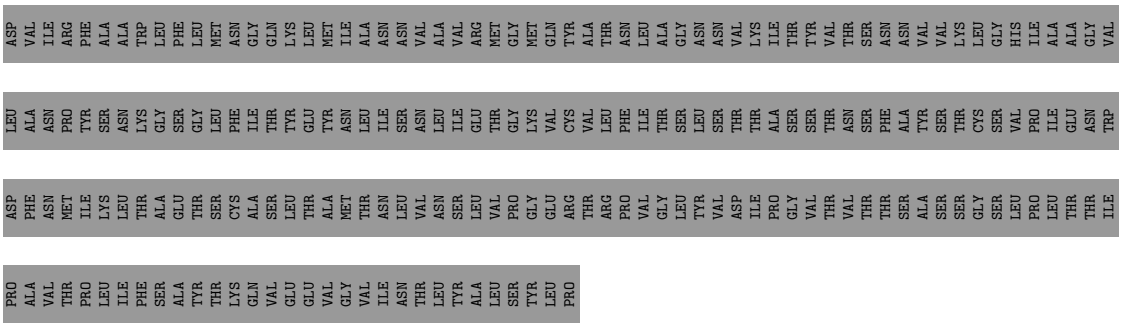


• Molecule 5: VP9

Chain r:

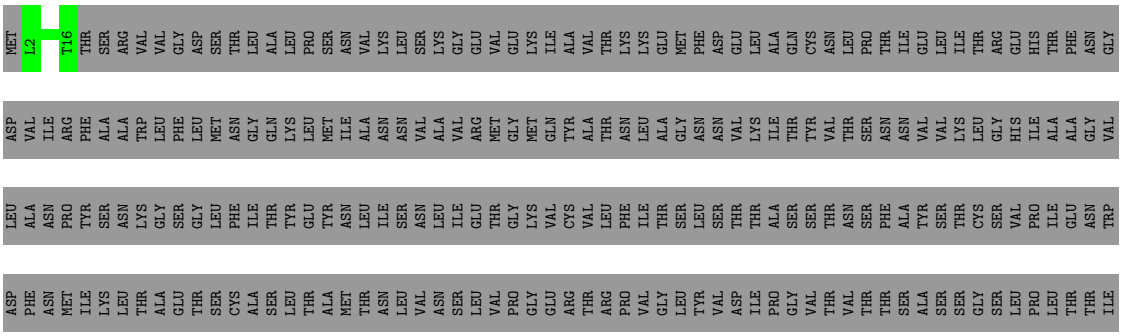






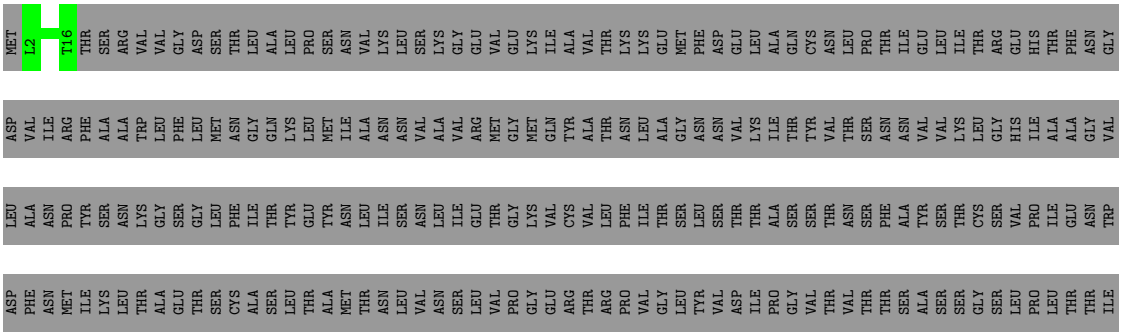
• Molecule 5: VP9

Chain s: 5% 95%



• Molecule 5: VP9

Chain t: 5% 95%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13225	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	1140.0, 1140.0, 1140.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.85, 2.85, 2.85	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/6179	0.47	0/8387
1	B	0.29	0/7361	0.47	0/9987
2	C	0.29	0/2333	0.48	0/3179
2	D	0.28	0/2322	0.47	0/3165
2	E	0.28	0/2322	0.47	0/3165
2	F	0.29	0/2322	0.49	0/3165
2	G	0.29	0/2322	0.49	0/3165
2	H	0.28	0/2333	0.48	0/3179
2	I	0.28	0/2322	0.49	0/3165
2	J	0.29	0/2333	0.48	0/3179
2	K	0.29	0/2322	0.47	0/3165
2	L	0.28	0/2315	0.47	0/3155
2	M	0.28	0/2322	0.48	0/3165
2	N	0.28	0/2322	0.48	0/3165
2	O	0.28	0/2322	0.46	0/3165
3	P	0.27	0/2050	0.47	0/2772
3	Q	0.27	0/2020	0.48	0/2730
4	R	0.27	0/4799	0.45	0/6515
4	S	0.27	0/4953	0.47	0/6725
4	T	0.27	0/4997	0.46	0/6787
5	r	0.22	0/116	0.46	0/154
5	s	0.23	0/116	0.50	0/154
5	t	0.23	0/116	0.53	0/154
All	All	0.28	0/62919	0.47	0/85542

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)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6045	0	5960	61	0
1	B	7210	0	7136	76	0
2	C	2288	0	2283	33	0
2	D	2277	0	2270	25	0
2	E	2277	0	2270	33	0
2	F	2277	0	2270	17	0
2	G	2277	0	2270	33	0
2	H	2288	0	2283	29	0
2	I	2277	0	2270	28	0
2	J	2288	0	2283	26	0
2	K	2277	0	2270	29	0
2	L	2270	0	2261	27	0
2	M	2277	0	2270	33	0
2	N	2277	0	2270	34	0
2	O	2277	0	2270	28	0
3	P	2014	0	2036	31	0
3	Q	1986	0	2008	36	0
4	R	4706	0	4649	97	0
4	S	4858	0	4796	87	0
4	T	4900	0	4835	113	0
5	r	117	0	130	0	0
5	s	117	0	130	0	0
5	t	117	0	130	0	0
All	All	61697	0	61350	826	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 826 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:210:ILE:CG2	4:T:212:GLN:HG2	1.85	1.05
2:I:168:ILE:HG12	2:I:268:TYR:CD2	1.93	1.03
4:T:258:HIS:CE1	4:T:356:GLN:HE22	1.79	0.99
2:H:182:LEU:HB3	2:H:196:TYR:CE2	1.97	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:517:HIS:CD2	4:T:519:LEU:HD23	1.97	0.99

There are no symmetry-related clashes.

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	747/955 (78%)	737 (99%)	10 (1%)	0	100	100
1	B	898/955 (94%)	880 (98%)	18 (2%)	0	100	100
2	C	297/302 (98%)	293 (99%)	4 (1%)	0	100	100
2	D	296/302 (98%)	287 (97%)	9 (3%)	0	100	100
2	E	296/302 (98%)	290 (98%)	6 (2%)	0	100	100
2	F	296/302 (98%)	290 (98%)	6 (2%)	0	100	100
2	G	296/302 (98%)	290 (98%)	6 (2%)	0	100	100
2	H	297/302 (98%)	292 (98%)	5 (2%)	0	100	100
2	I	296/302 (98%)	286 (97%)	10 (3%)	0	100	100
2	J	297/302 (98%)	291 (98%)	6 (2%)	0	100	100
2	K	296/302 (98%)	293 (99%)	3 (1%)	0	100	100
2	L	295/302 (98%)	286 (97%)	9 (3%)	0	100	100
2	M	296/302 (98%)	291 (98%)	5 (2%)	0	100	100
2	N	296/302 (98%)	289 (98%)	7 (2%)	0	100	100
2	O	296/302 (98%)	291 (98%)	5 (2%)	0	100	100
3	P	247/249 (99%)	245 (99%)	2 (1%)	0	100	100
3	Q	242/249 (97%)	233 (96%)	9 (4%)	0	100	100
4	R	599/628 (95%)	593 (99%)	6 (1%)	0	100	100
4	S	620/628 (99%)	609 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	T	625/628 (100%)	609 (97%)	16 (3%)	0	100	100
5	r	13/283 (5%)	13 (100%)	0	0	100	100
5	s	13/283 (5%)	13 (100%)	0	0	100	100
5	t	13/283 (5%)	13 (100%)	0	0	100	100
All	All	7867/9067 (87%)	7714 (98%)	153 (2%)	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	A	673/846 (80%)	673 (100%)	0	100	100
1	B	803/846 (95%)	803 (100%)	0	100	100
2	C	249/252 (99%)	249 (100%)	0	100	100
2	D	248/252 (98%)	248 (100%)	0	100	100
2	E	248/252 (98%)	248 (100%)	0	100	100
2	F	248/252 (98%)	248 (100%)	0	100	100
2	G	248/252 (98%)	248 (100%)	0	100	100
2	H	249/252 (99%)	249 (100%)	0	100	100
2	I	248/252 (98%)	248 (100%)	0	100	100
2	J	249/252 (99%)	249 (100%)	0	100	100
2	K	248/252 (98%)	248 (100%)	0	100	100
2	L	247/252 (98%)	247 (100%)	0	100	100
2	M	248/252 (98%)	248 (100%)	0	100	100
2	N	248/252 (98%)	248 (100%)	0	100	100
2	O	248/252 (98%)	248 (100%)	0	100	100
3	P	225/225 (100%)	225 (100%)	0	100	100
3	Q	223/225 (99%)	223 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	509/532 (96%)	509 (100%)	0	100	100
4	S	527/532 (99%)	527 (100%)	0	100	100
4	T	531/532 (100%)	531 (100%)	0	100	100
5	r	14/245 (6%)	14 (100%)	0	100	100
5	s	14/245 (6%)	14 (100%)	0	100	100
5	t	14/245 (6%)	14 (100%)	0	100	100
All	All	6759/7749 (87%)	6759 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
4	T	258	HIS
4	T	99	GLN
4	S	322	ASN
4	T	97	GLN
4	S	139	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

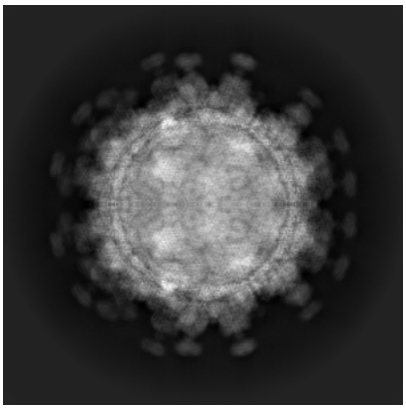
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37379. These allow visual inspection of the internal detail of the map and identification of artifacts.

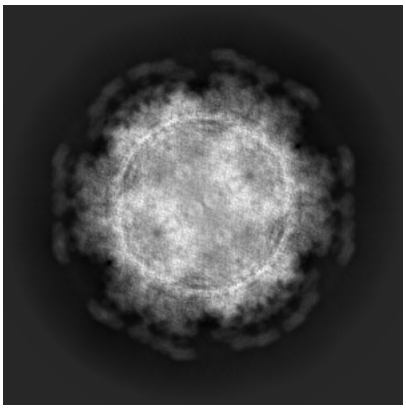
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

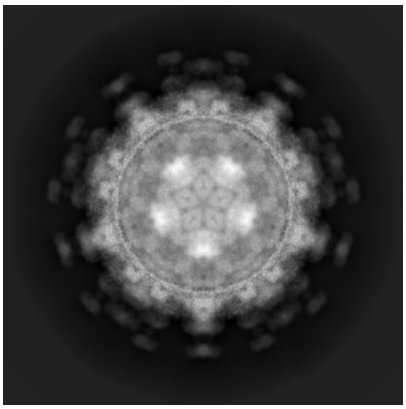
6.1.1 Primary map



X

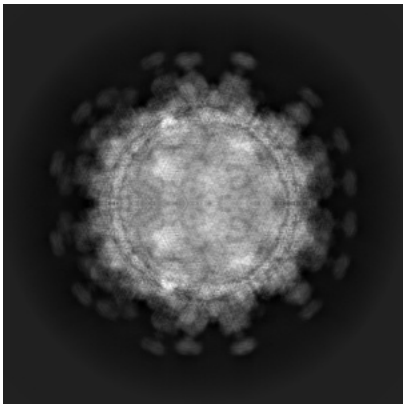


Y

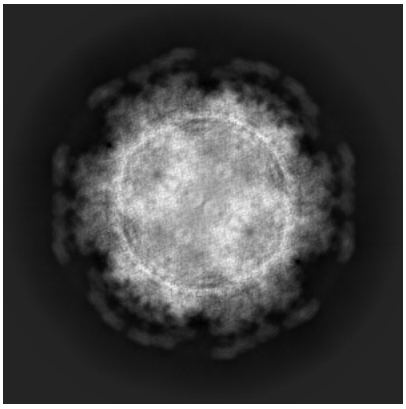


Z

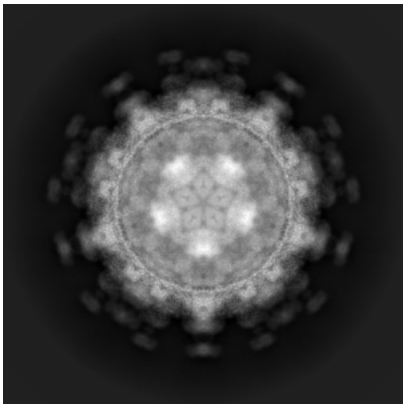
6.1.2 Raw map



X



Y

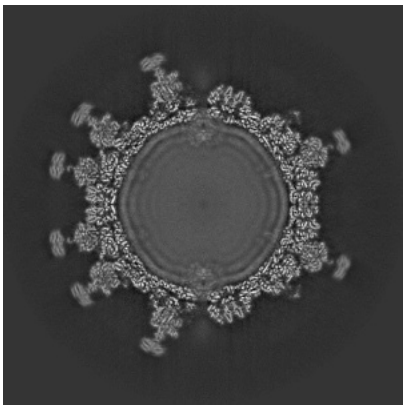


Z

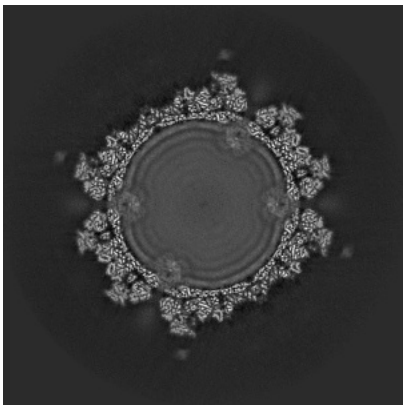
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

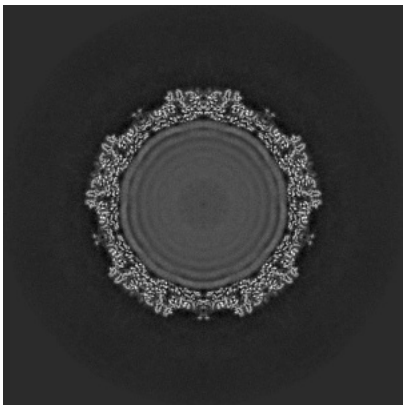
6.2.1 Primary map



X Index: 200

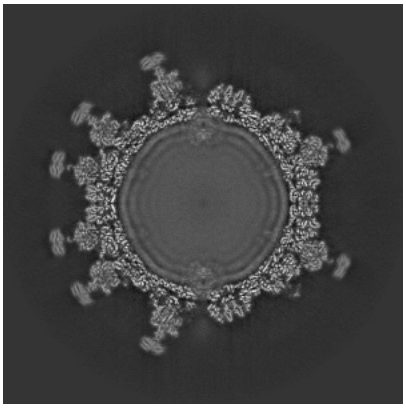


Y Index: 200

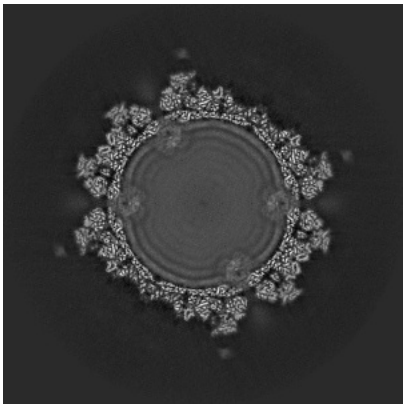


Z Index: 200

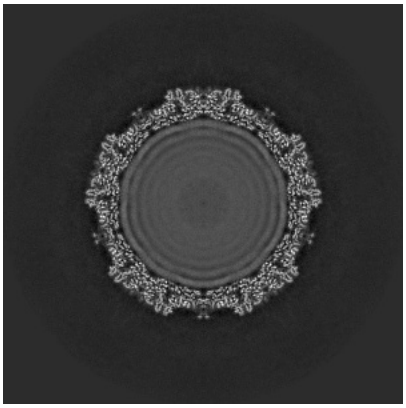
6.2.2 Raw map



X Index: 200



Y Index: 200

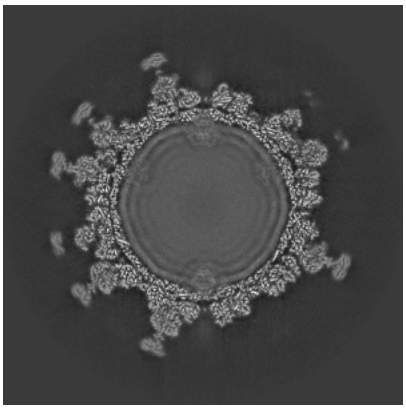


Z Index: 200

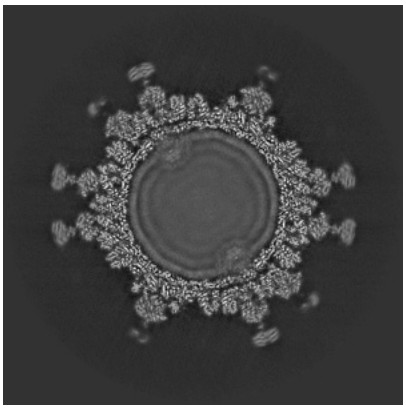
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

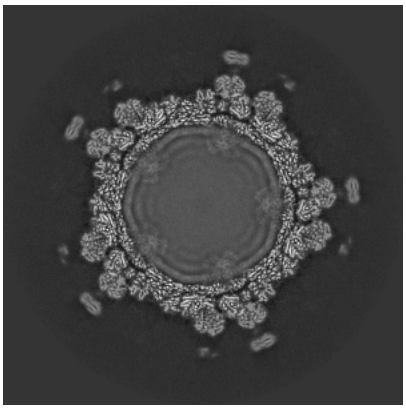
6.3.1 Primary map



X Index: 204

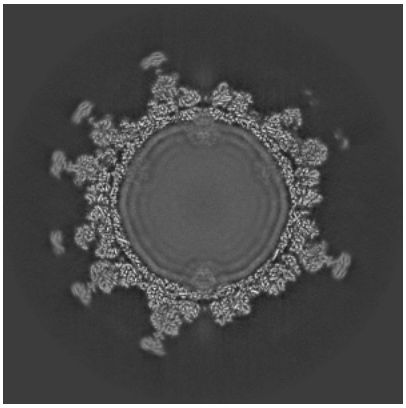


Y Index: 239

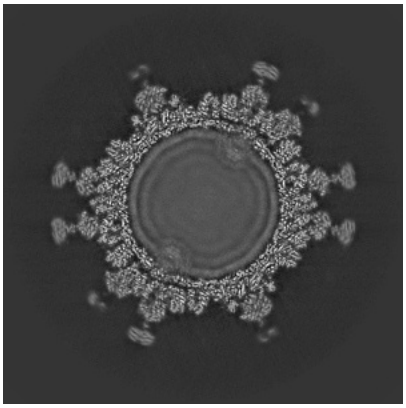


Z Index: 227

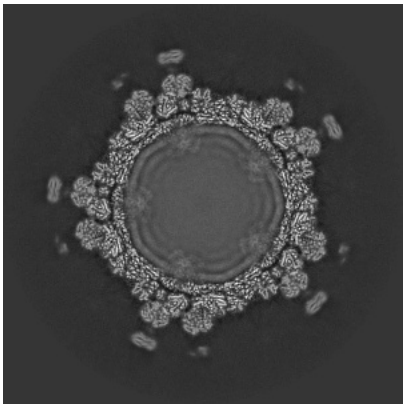
6.3.2 Raw map



X Index: 196



Y Index: 239

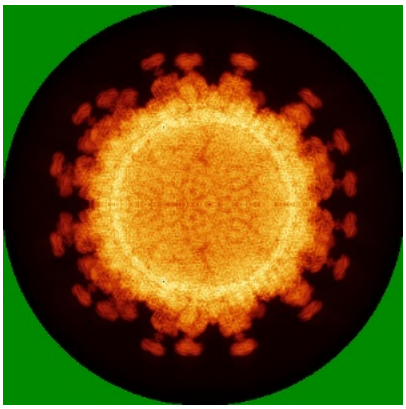


Z Index: 227

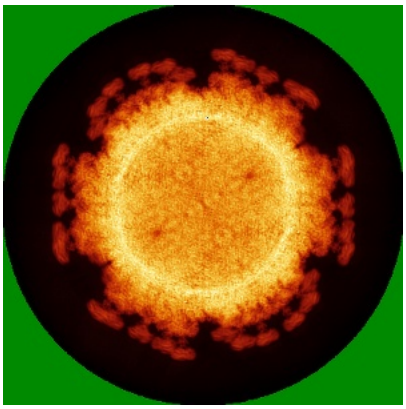
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

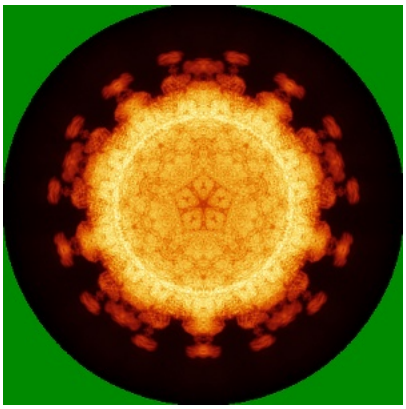
6.4.1 Primary map



X

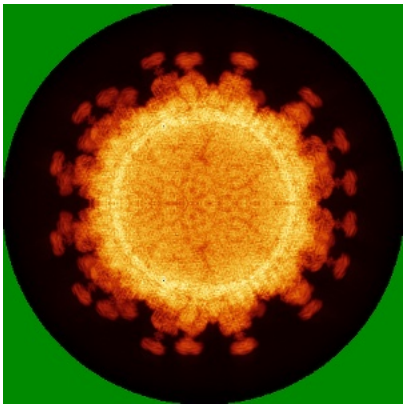


Y

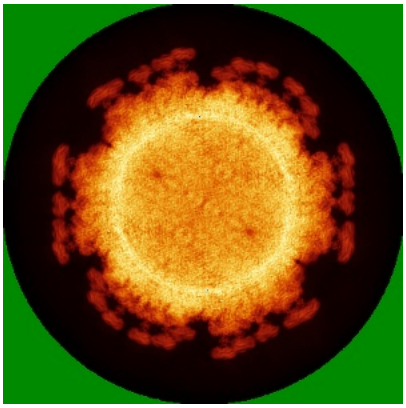


Z

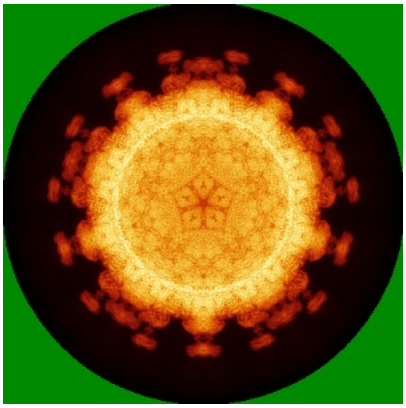
6.4.2 Raw map



X



Y

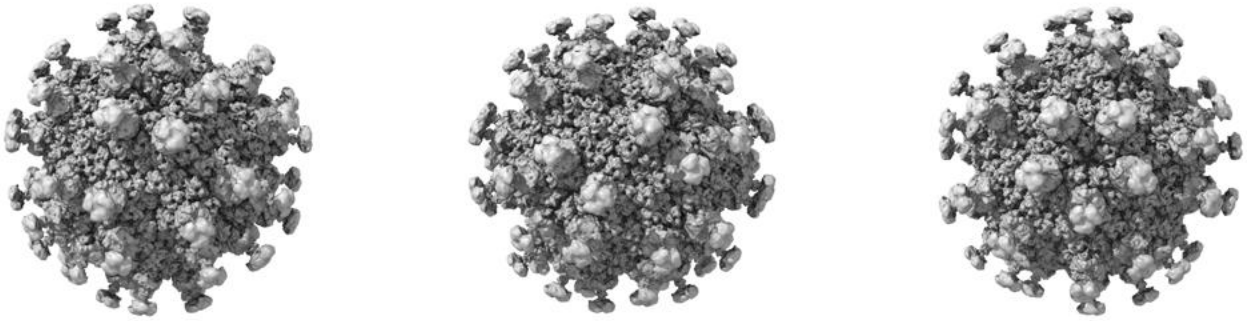


Z

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)

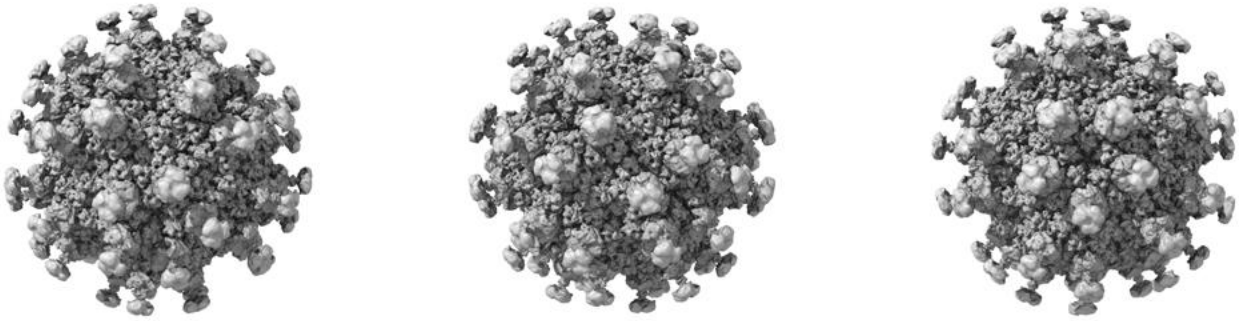
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. 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



X Y Z

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.

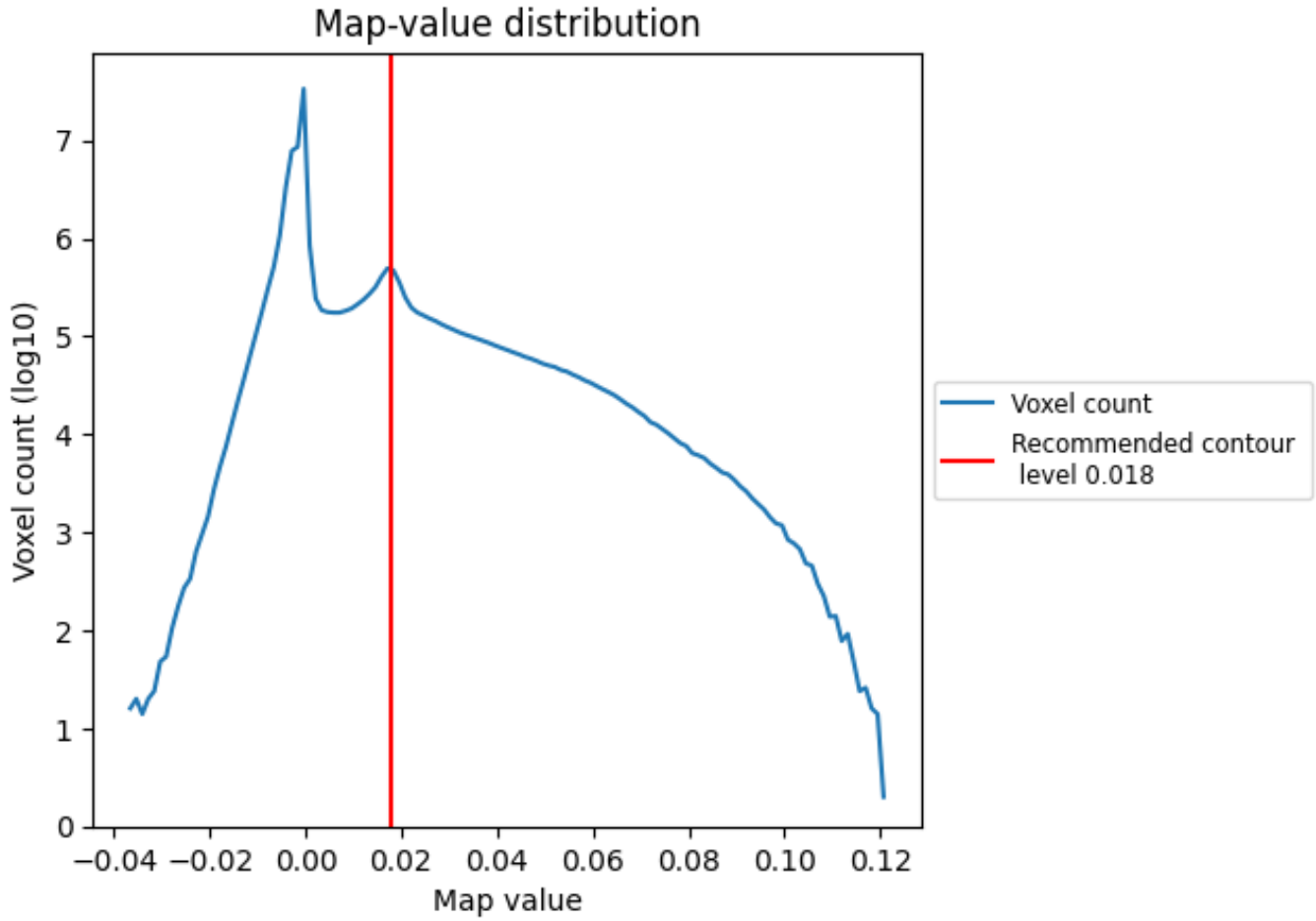
6.6 Mask visualisation (i)

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

7 Map analysis

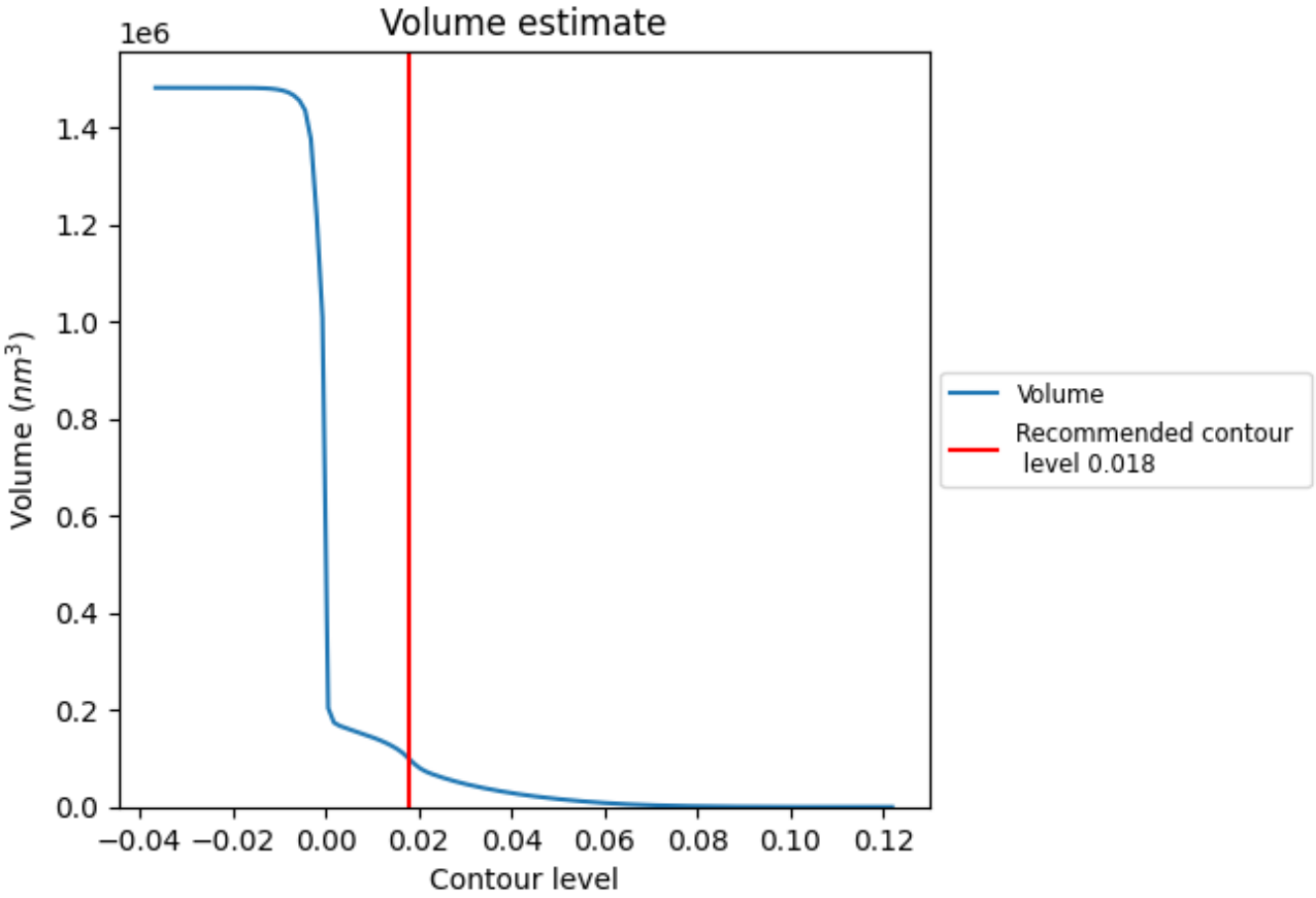
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

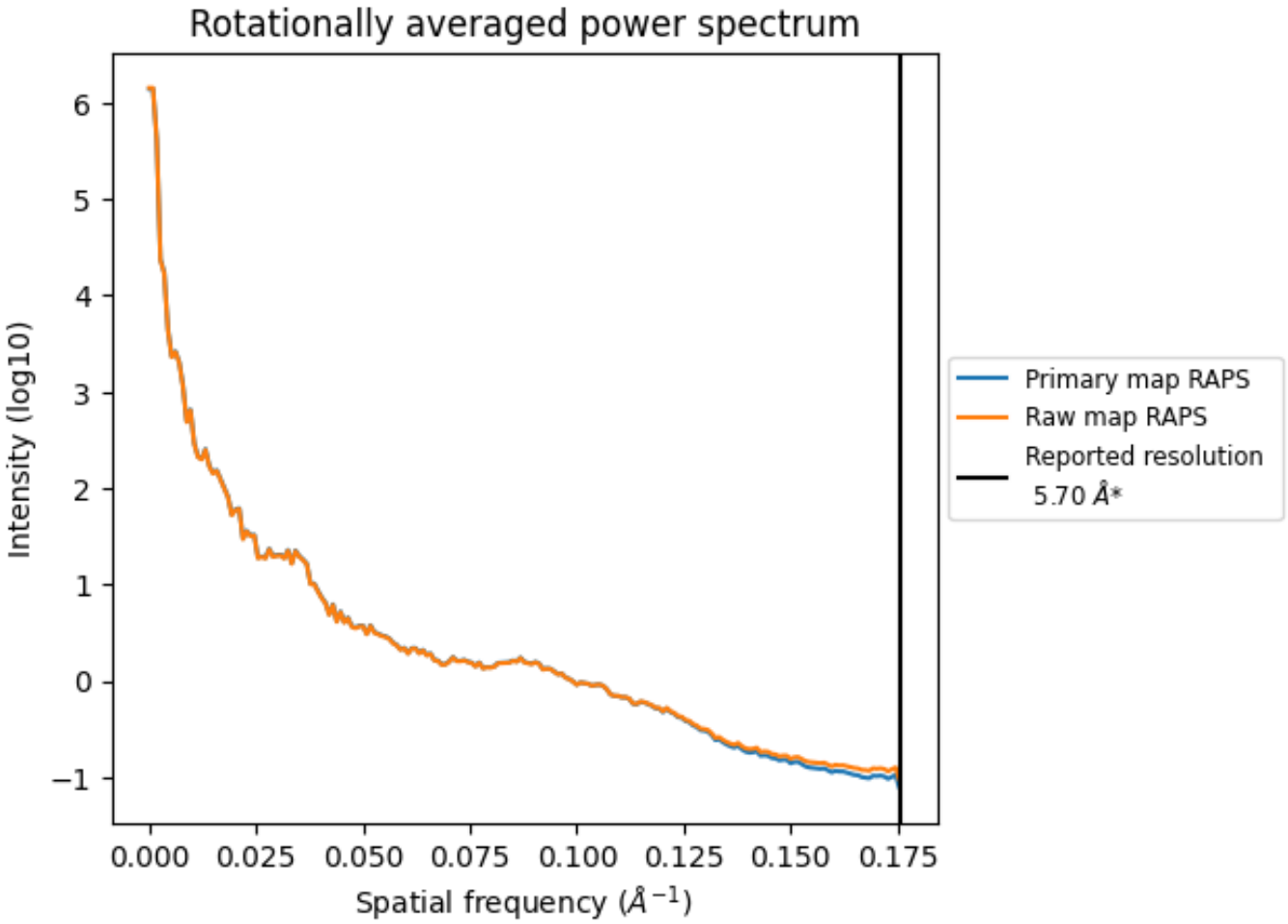
7.2 Volume estimate (i)



The volume at the recommended contour level is 99216 nm^3; this corresponds to an approximate mass of 89624 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)

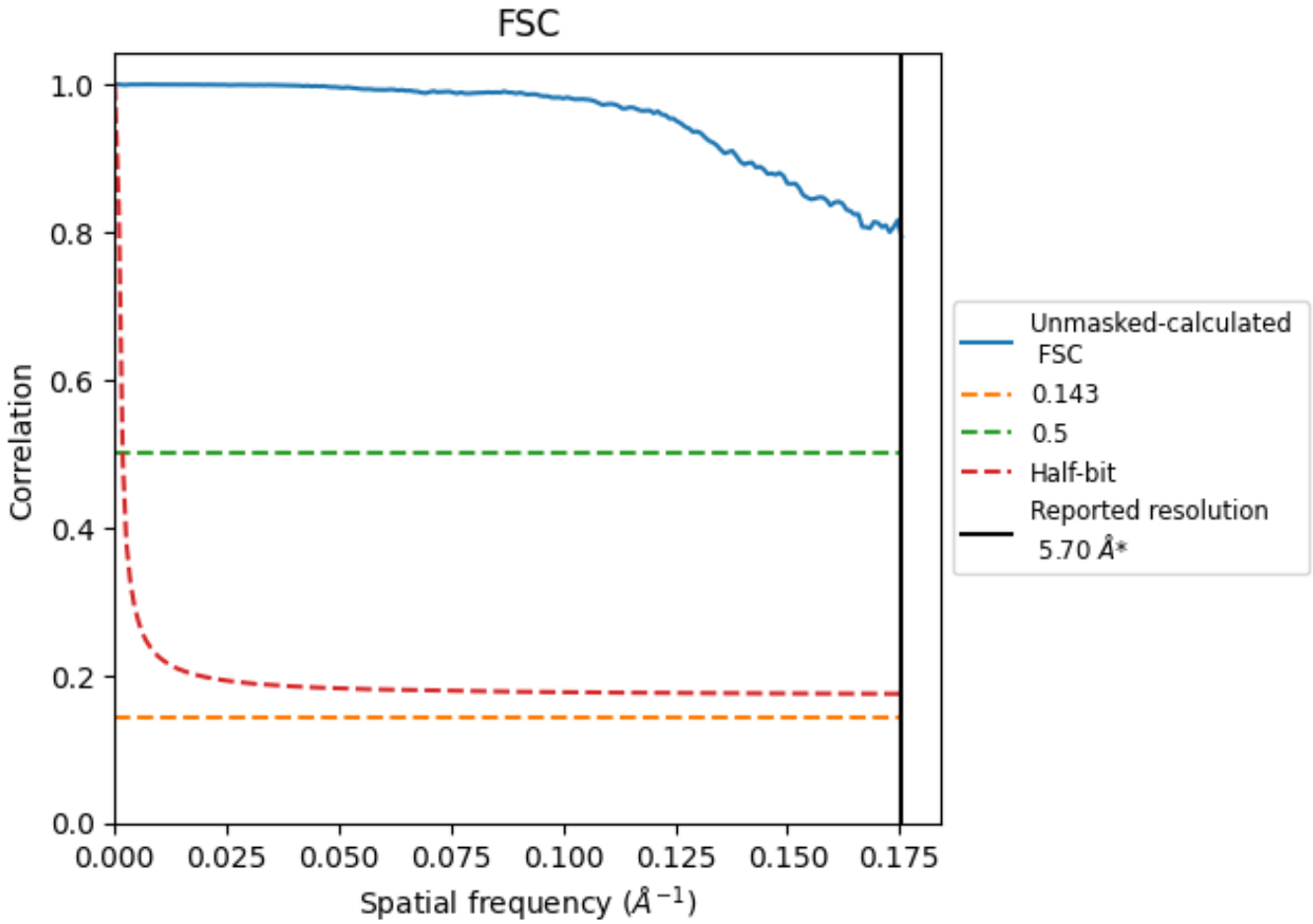


*Reported resolution corresponds to spatial frequency of 0.175 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.175 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

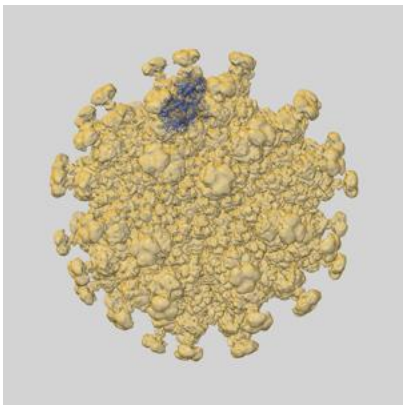
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

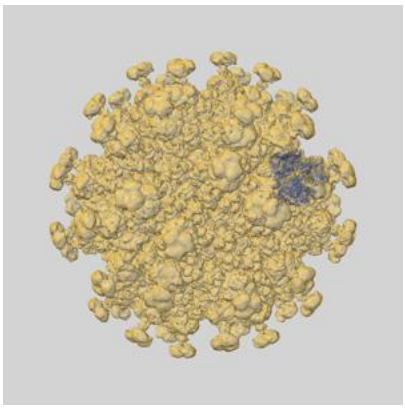
This section contains information regarding the fit between EMDB map EMD-37379 and PDB model 8W9Q. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

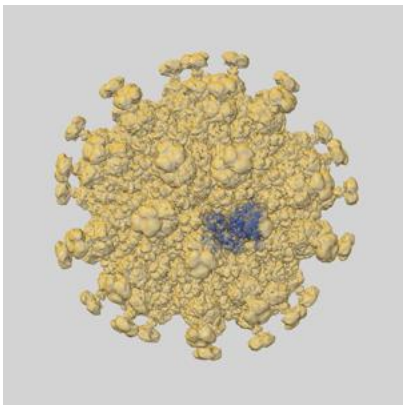
9.1.1 Map-model overlay



X

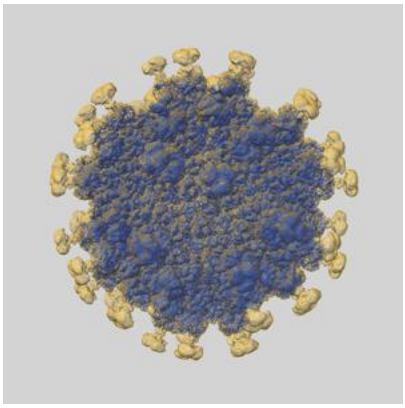


Y

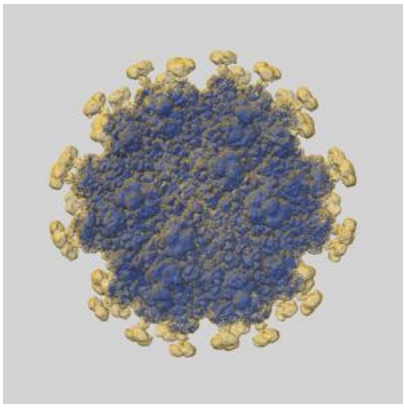


Z

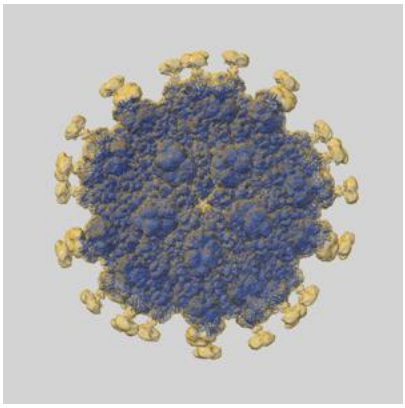
9.1.2 Map-model assembly overlay



X



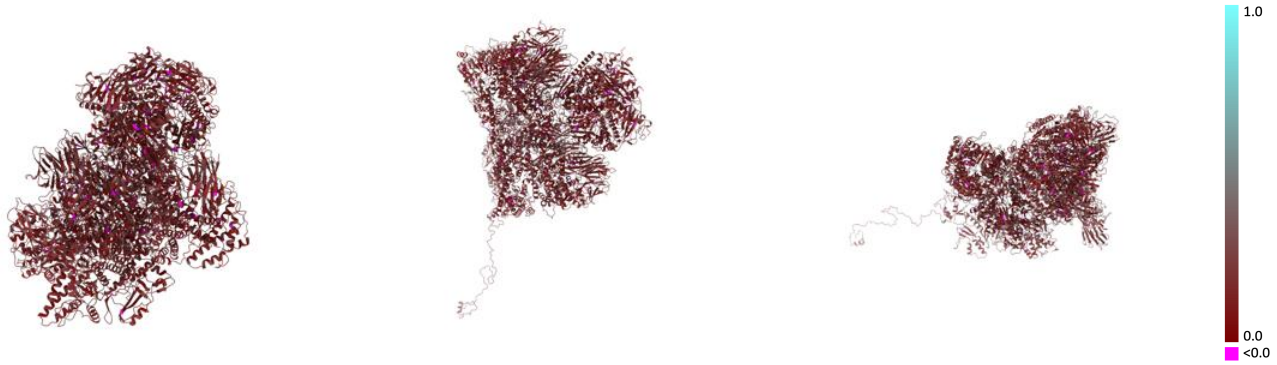
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

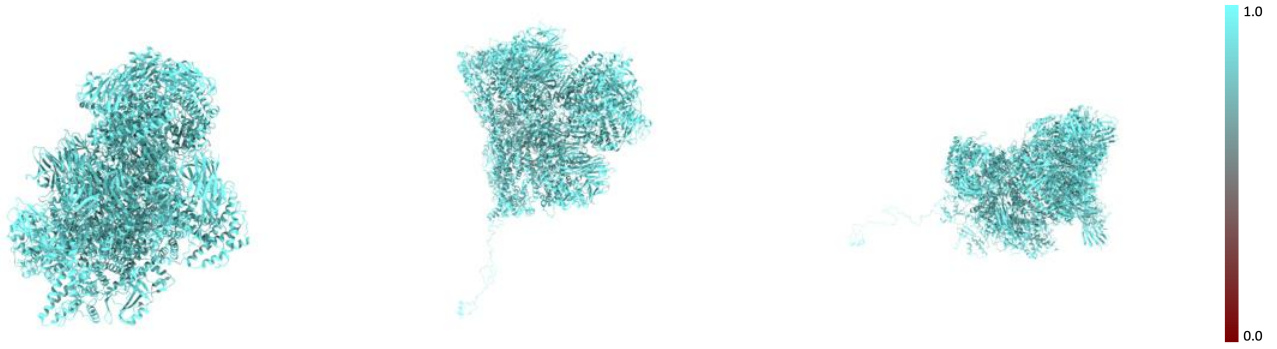
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

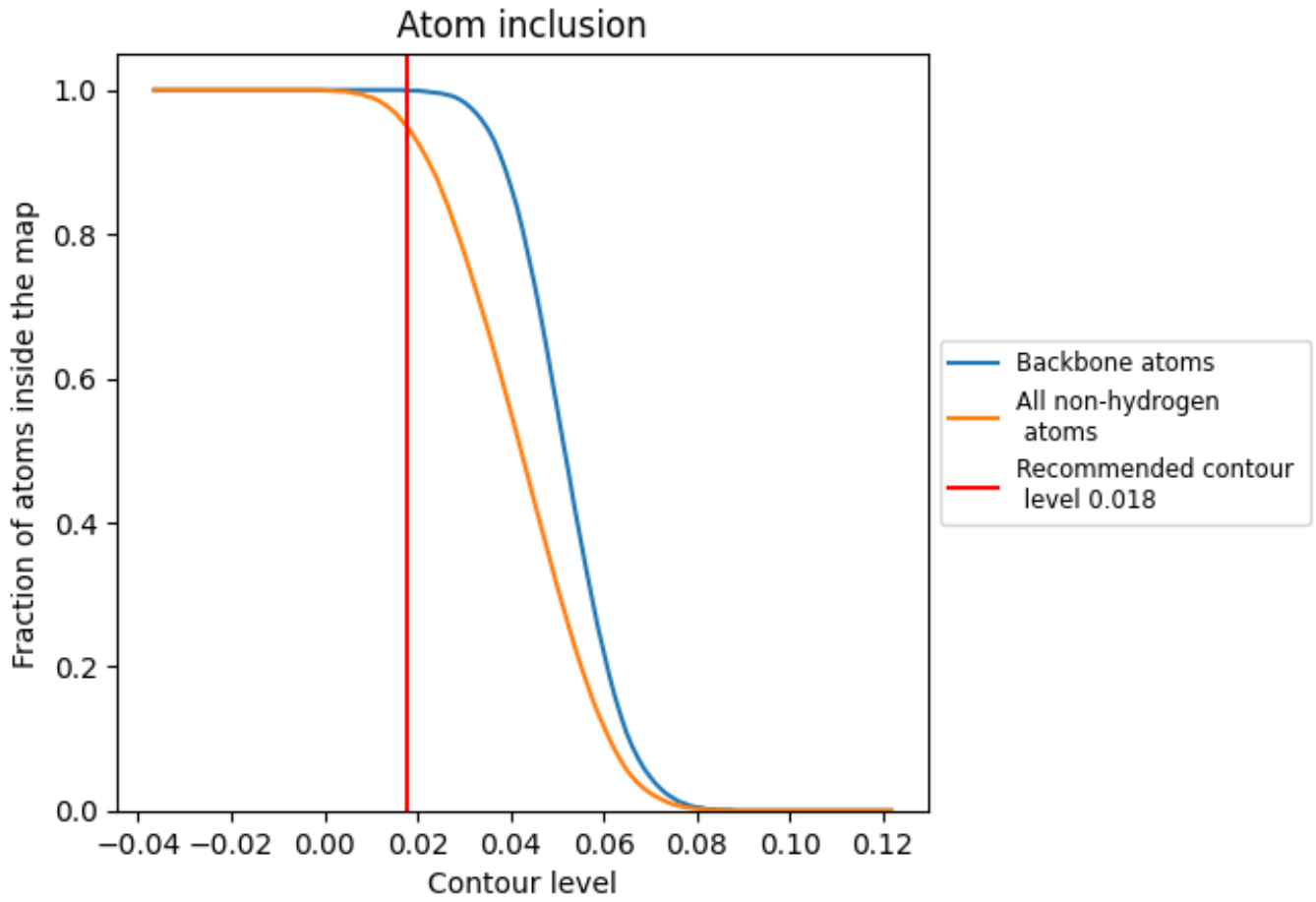
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 95% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9480	0.1970
A	0.9310	0.2000
B	0.9260	0.2030
C	0.9560	0.2000
D	0.9540	0.2010
E	0.9650	0.2040
F	0.9490	0.1990
G	0.9530	0.2040
H	0.9420	0.1910
I	0.9480	0.2040
J	0.9570	0.2000
K	0.9500	0.1990
L	0.9710	0.1990
M	0.9600	0.1980
N	0.9660	0.1970
O	0.9490	0.2070
P	0.9320	0.1950
Q	0.9330	0.1950
R	0.9510	0.1840
S	0.9570	0.1870
T	0.9560	0.1920
r	0.9480	0.1700
s	0.9740	0.1380
t	0.9650	0.1800