Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 10:48 PM EST

PDB ID	:	6V7B
EMDB ID	:	EMD-21094
Title	:	Cryo-EM reconstruction of Pyrobaculum filamentous virus 2 (PFV2)
Authors	:	Wang, F.; Baquero, D.P.; Su, Z.; Prangishvili, D.; Krupovic, M.; Egelman, E.H.
Deposited on	:	2019-12-08
Resolution	:	3.40 Å(reported)

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

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

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

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

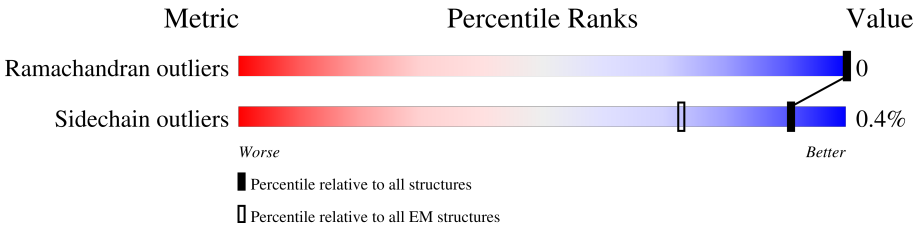
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	323	87% 13%
2	2	323	74% 26%
3	A	129	91% 8%
3	B	129	91% 8%
3	C	129	91% 8%
3	D	129	92% 8%
3	E	129	92% 8%
3	F	129	92% 8%
3	G	129	91% 8%

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Mol	Chain	Length	Quality of chain
3	H	129	92% 8%
3	I	129	91% 8%
3	J	129	92% 8%
3	K	129	92% 8%
3	L	129	91% 8%
3	M	129	91% 8%
3	N	129	91% 8%
3	O	129	91% 8%
3	P	129	92% 8%
3	Q	129	91% 8%
3	R	129	91% 8%
3	S	129	92% 8%
3	T	129	91% 8%
3	U	129	92% 8%
3	V	129	92% 8%
3	W	129	91% 8%
4	a	145	87% 13%
4	b	145	87% 13%
4	c	145	87% 13%
4	d	145	87% 13%
4	e	145	87% 13%
4	f	145	87% 13%
4	g	145	86% 13%
4	h	145	87% 13%
4	i	145	87% 13%

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Mol	Chain	Length	Quality of chain
4	j	145	87% 13%
4	k	145	87% 13%
4	l	145	87% 13%
4	m	145	87% 13%
4	n	145	87% 13%
4	o	145	87% 13%
4	p	145	87% 13%
4	q	145	87% 13%
4	r	145	87% 13%
4	s	145	87% 13%
4	t	145	87% 13%
4	u	145	87% 13%
4	v	145	87% 13%
4	w	145	87% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 58277 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 DNA chain called A-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	323	Total	C	N	O	P	0	0
			6622	3230	1132	1937	323		

- Molecule 2 is a DNA chain called A-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	323	Total	C	N	O	P	0	0
			6621	3230	1129	1939	323		

- Molecule 3 is a protein called Structural protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	B	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	C	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	D	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	E	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	F	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	G	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	H	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	I	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	J	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	K	119	Total	C	N	O	S	0	0
			974	618	175	177	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	M	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	N	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	O	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	P	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	Q	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	R	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	S	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	T	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	U	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	V	119	Total	C	N	O	S	0	0
			974	618	175	177	4		
3	W	119	Total	C	N	O	S	0	0
			974	618	175	177	4		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLU	GLY	conflict	UNP A0A140F3K6
A	54	ARG	LYS	conflict	UNP A0A140F3K6
A	115	THR	ILE	conflict	UNP A0A140F3K6
B	43	GLU	GLY	conflict	UNP A0A140F3K6
B	54	ARG	LYS	conflict	UNP A0A140F3K6
B	115	THR	ILE	conflict	UNP A0A140F3K6
C	43	GLU	GLY	conflict	UNP A0A140F3K6
C	54	ARG	LYS	conflict	UNP A0A140F3K6
C	115	THR	ILE	conflict	UNP A0A140F3K6
D	43	GLU	GLY	conflict	UNP A0A140F3K6
D	54	ARG	LYS	conflict	UNP A0A140F3K6
D	115	THR	ILE	conflict	UNP A0A140F3K6
E	43	GLU	GLY	conflict	UNP A0A140F3K6
E	54	ARG	LYS	conflict	UNP A0A140F3K6
E	115	THR	ILE	conflict	UNP A0A140F3K6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	43	GLU	GLY	conflict	UNP A0A140F3K6
F	54	ARG	LYS	conflict	UNP A0A140F3K6
F	115	THR	ILE	conflict	UNP A0A140F3K6
G	43	GLU	GLY	conflict	UNP A0A140F3K6
G	54	ARG	LYS	conflict	UNP A0A140F3K6
G	115	THR	ILE	conflict	UNP A0A140F3K6
H	43	GLU	GLY	conflict	UNP A0A140F3K6
H	54	ARG	LYS	conflict	UNP A0A140F3K6
H	115	THR	ILE	conflict	UNP A0A140F3K6
I	43	GLU	GLY	conflict	UNP A0A140F3K6
I	54	ARG	LYS	conflict	UNP A0A140F3K6
I	115	THR	ILE	conflict	UNP A0A140F3K6
J	43	GLU	GLY	conflict	UNP A0A140F3K6
J	54	ARG	LYS	conflict	UNP A0A140F3K6
J	115	THR	ILE	conflict	UNP A0A140F3K6
K	43	GLU	GLY	conflict	UNP A0A140F3K6
K	54	ARG	LYS	conflict	UNP A0A140F3K6
K	115	THR	ILE	conflict	UNP A0A140F3K6
L	43	GLU	GLY	conflict	UNP A0A140F3K6
L	54	ARG	LYS	conflict	UNP A0A140F3K6
L	115	THR	ILE	conflict	UNP A0A140F3K6
M	43	GLU	GLY	conflict	UNP A0A140F3K6
M	54	ARG	LYS	conflict	UNP A0A140F3K6
M	115	THR	ILE	conflict	UNP A0A140F3K6
N	43	GLU	GLY	conflict	UNP A0A140F3K6
N	54	ARG	LYS	conflict	UNP A0A140F3K6
N	115	THR	ILE	conflict	UNP A0A140F3K6
O	43	GLU	GLY	conflict	UNP A0A140F3K6
O	54	ARG	LYS	conflict	UNP A0A140F3K6
O	115	THR	ILE	conflict	UNP A0A140F3K6
P	43	GLU	GLY	conflict	UNP A0A140F3K6
P	54	ARG	LYS	conflict	UNP A0A140F3K6
P	115	THR	ILE	conflict	UNP A0A140F3K6
Q	43	GLU	GLY	conflict	UNP A0A140F3K6
Q	54	ARG	LYS	conflict	UNP A0A140F3K6
Q	115	THR	ILE	conflict	UNP A0A140F3K6
R	43	GLU	GLY	conflict	UNP A0A140F3K6
R	54	ARG	LYS	conflict	UNP A0A140F3K6
R	115	THR	ILE	conflict	UNP A0A140F3K6
S	43	GLU	GLY	conflict	UNP A0A140F3K6
S	54	ARG	LYS	conflict	UNP A0A140F3K6
S	115	THR	ILE	conflict	UNP A0A140F3K6

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Chain	Residue	Modelled	Actual	Comment	Reference
T	43	GLU	GLY	conflict	UNP A0A140F3K6
T	54	ARG	LYS	conflict	UNP A0A140F3K6
T	115	THR	ILE	conflict	UNP A0A140F3K6
U	43	GLU	GLY	conflict	UNP A0A140F3K6
U	54	ARG	LYS	conflict	UNP A0A140F3K6
U	115	THR	ILE	conflict	UNP A0A140F3K6
V	43	GLU	GLY	conflict	UNP A0A140F3K6
V	54	ARG	LYS	conflict	UNP A0A140F3K6
V	115	THR	ILE	conflict	UNP A0A140F3K6
W	43	GLU	GLY	conflict	UNP A0A140F3K6
W	54	ARG	LYS	conflict	UNP A0A140F3K6
W	115	THR	ILE	conflict	UNP A0A140F3K6

- Molecule 4 is a protein called Structural protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	b	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	c	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	d	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	e	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	f	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	g	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	h	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	i	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	j	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	k	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	l	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	m	126	Total	C	N	O	S	0	0
			984	620	178	179	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	o	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	p	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	q	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	r	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	s	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	t	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	u	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	v	126	Total	C	N	O	S	0	0
			984	620	178	179	7		
4	w	126	Total	C	N	O	S	0	0
			984	620	178	179	7		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	28	GLU	GLY	conflict	UNP A0A140F3K7
b	28	GLU	GLY	conflict	UNP A0A140F3K7
c	28	GLU	GLY	conflict	UNP A0A140F3K7
d	28	GLU	GLY	conflict	UNP A0A140F3K7
e	28	GLU	GLY	conflict	UNP A0A140F3K7
f	28	GLU	GLY	conflict	UNP A0A140F3K7
g	28	GLU	GLY	conflict	UNP A0A140F3K7
h	28	GLU	GLY	conflict	UNP A0A140F3K7
i	28	GLU	GLY	conflict	UNP A0A140F3K7
j	28	GLU	GLY	conflict	UNP A0A140F3K7
k	28	GLU	GLY	conflict	UNP A0A140F3K7
l	28	GLU	GLY	conflict	UNP A0A140F3K7
m	28	GLU	GLY	conflict	UNP A0A140F3K7
n	28	GLU	GLY	conflict	UNP A0A140F3K7
o	28	GLU	GLY	conflict	UNP A0A140F3K7
p	28	GLU	GLY	conflict	UNP A0A140F3K7
q	28	GLU	GLY	conflict	UNP A0A140F3K7
r	28	GLU	GLY	conflict	UNP A0A140F3K7
s	28	GLU	GLY	conflict	UNP A0A140F3K7

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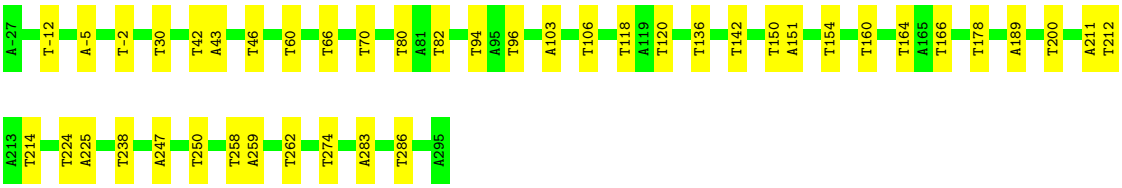
Chain	Residue	Modelled	Actual	Comment	Reference
t	28	GLU	GLY	conflict	UNP A0A140F3K7
u	28	GLU	GLY	conflict	UNP A0A140F3K7
v	28	GLU	GLY	conflict	UNP A0A140F3K7
w	28	GLU	GLY	conflict	UNP A0A140F3K7

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: A-DNA

Chain 1:

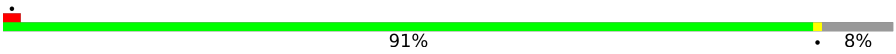


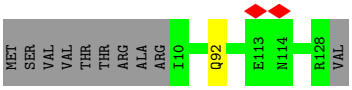
• Molecule 2: A-DNA

Chain 2:

• Molecule 3: Structural protein VP1

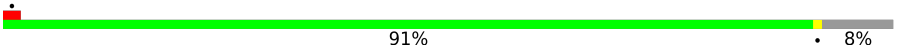
Chain A:

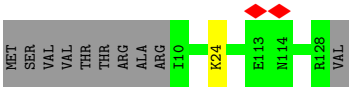




• Molecule 3: Structural protein VP1

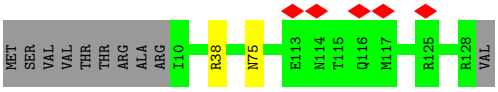
Chain B:





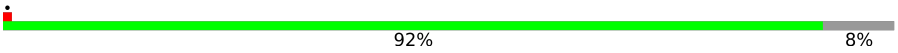
• Molecule 3: Structural protein VP1

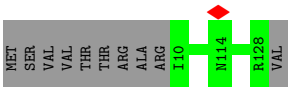
Chain C:



• Molecule 3: Structural protein VP1

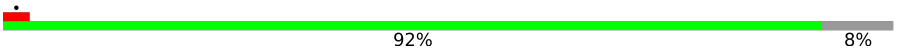
Chain D:

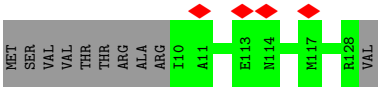




• Molecule 3: Structural protein VP1

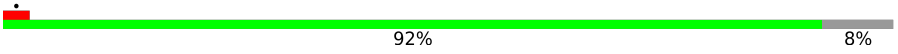
Chain E:

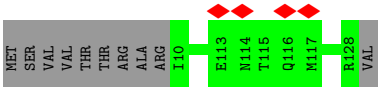




• Molecule 3: Structural protein VP1

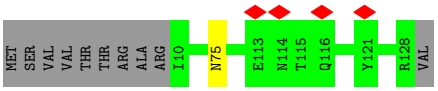
Chain F:





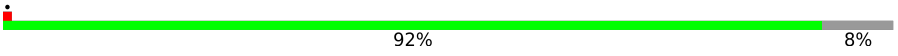
• Molecule 3: Structural protein VP1

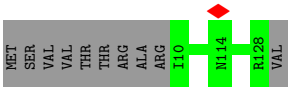
Chain G:



• Molecule 3: Structural protein VP1

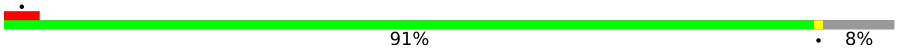
Chain H:

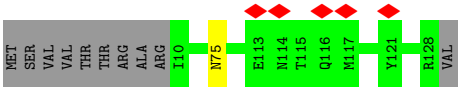




• Molecule 3: Structural protein VP1

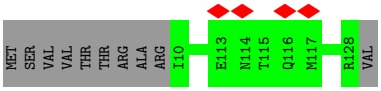
Chain I:





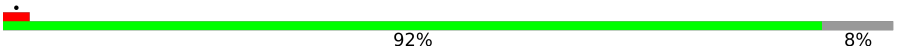
• Molecule 3: Structural protein VP1

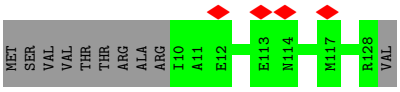
Chain J:



• Molecule 3: Structural protein VP1

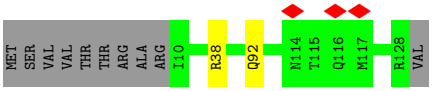
Chain K:





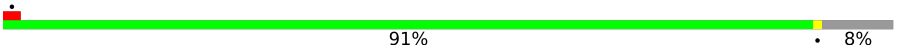
• Molecule 3: Structural protein VP1

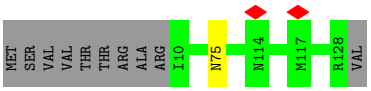
Chain L:



• Molecule 3: Structural protein VP1

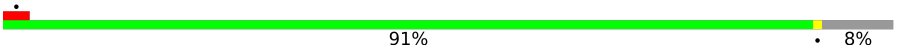
Chain M:

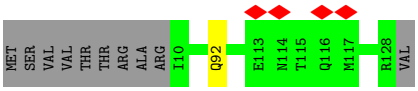




• Molecule 3: Structural protein VP1

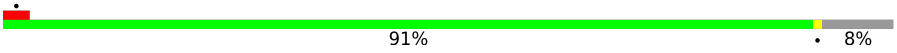
Chain N:

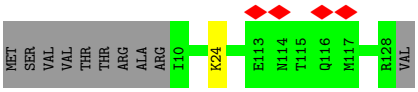




• Molecule 3: Structural protein VP1

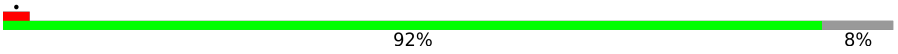
Chain O:

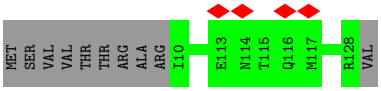




• Molecule 3: Structural protein VP1

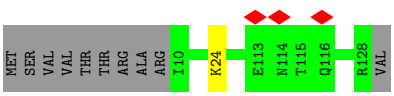
Chain P:





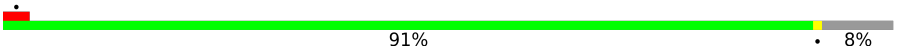
• Molecule 3: Structural protein VP1

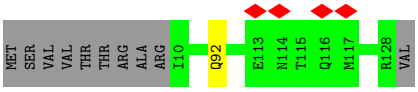
Chain Q:



• Molecule 3: Structural protein VP1

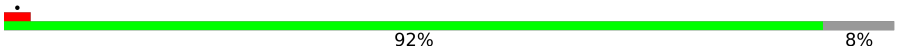
Chain R:

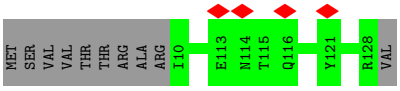




• Molecule 3: Structural protein VP1

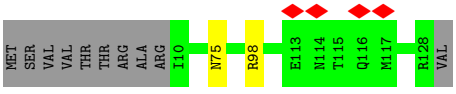
Chain S:





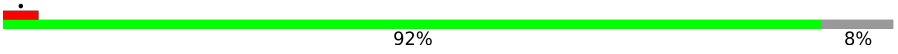
• Molecule 3: Structural protein VP1

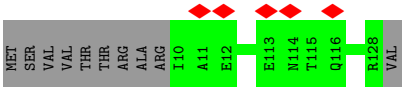
Chain T:



• Molecule 3: Structural protein VP1

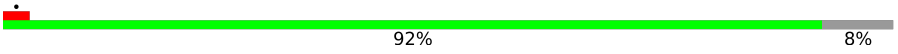
Chain U:

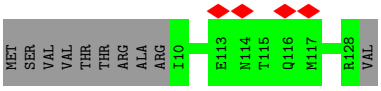




• Molecule 3: Structural protein VP1

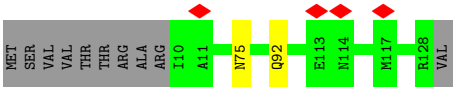
Chain V:





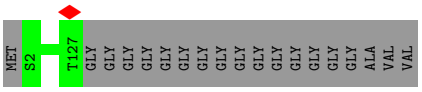
• Molecule 3: Structural protein VP1

Chain W:



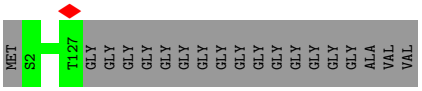
• Molecule 4: Structural protein VP2

Chain a:



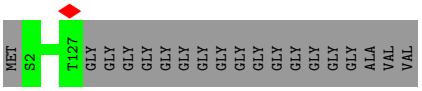
• Molecule 4: Structural protein VP2

Chain b:



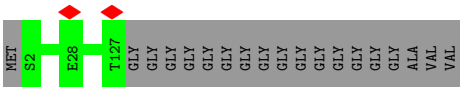
• Molecule 4: Structural protein VP2

Chain c:



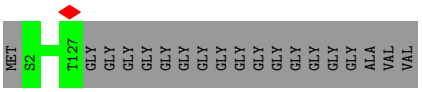
• Molecule 4: Structural protein VP2

Chain d:



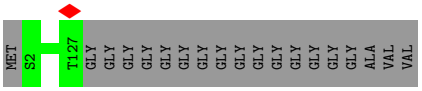
• Molecule 4: Structural protein VP2

Chain e:



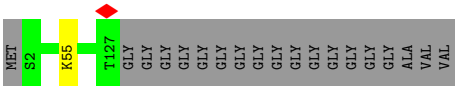
• Molecule 4: Structural protein VP2

Chain f:



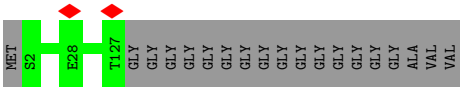
• Molecule 4: Structural protein VP2

Chain g:



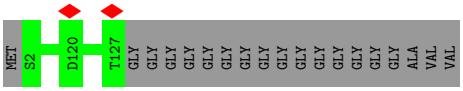
• Molecule 4: Structural protein VP2

Chain h:



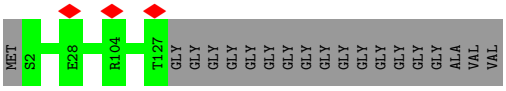
• Molecule 4: Structural protein VP2

Chain i:



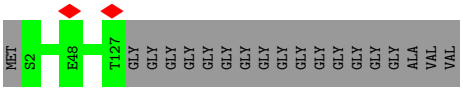
• Molecule 4: Structural protein VP2

Chain j:



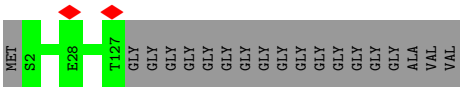
• Molecule 4: Structural protein VP2

Chain k:



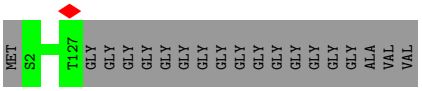
• Molecule 4: Structural protein VP2

Chain l:



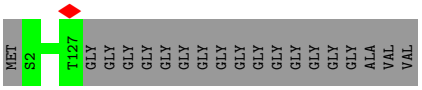
• Molecule 4: Structural protein VP2

Chain m:



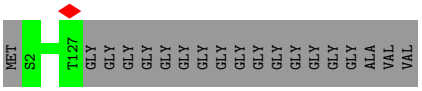
• Molecule 4: Structural protein VP2

Chain n:



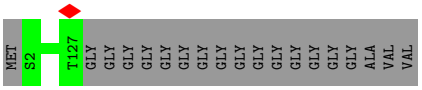
• Molecule 4: Structural protein VP2

Chain o:



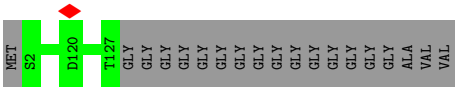
• Molecule 4: Structural protein VP2

Chain p:



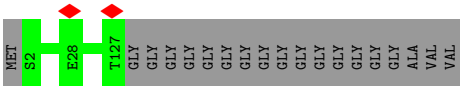
• Molecule 4: Structural protein VP2

Chain q:



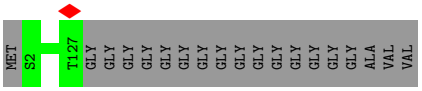
• Molecule 4: Structural protein VP2

Chain r:



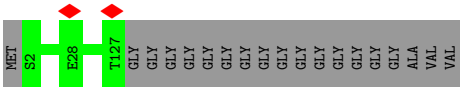
• Molecule 4: Structural protein VP2

Chain s:



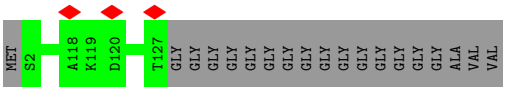
• Molecule 4: Structural protein VP2

Chain t:



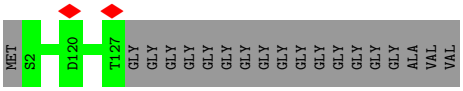
• Molecule 4: Structural protein VP2

Chain u:



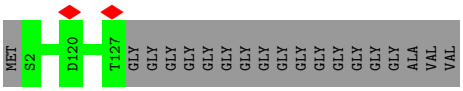
• Molecule 4: Structural protein VP2

Chain v:



• Molecule 4: Structural protein VP2

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=22.9482°, rise=2.864 Å, axial sym=C1	Depositor
Number of segments used	186576	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.065	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	448.0, 448.0, 448.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	1	0.99	0/7429	1.23	44/11464 (0.4%)
2	2	1.05	0/7427	1.32	83/11461 (0.7%)
3	A	0.36	0/990	0.48	0/1336
3	B	0.36	0/990	0.50	0/1336
3	C	0.37	0/990	0.50	0/1336
3	D	0.37	0/990	0.49	0/1336
3	E	0.36	0/990	0.49	0/1336
3	F	0.37	0/990	0.48	0/1336
3	G	0.36	0/990	0.49	0/1336
3	H	0.37	0/990	0.50	0/1336
3	I	0.35	0/990	0.49	0/1336
3	J	0.37	0/990	0.51	0/1336
3	K	0.36	0/990	0.52	0/1336
3	L	0.37	0/990	0.51	0/1336
3	M	0.36	0/990	0.49	0/1336
3	N	0.37	0/990	0.48	0/1336
3	O	0.35	0/990	0.48	0/1336
3	P	0.39	0/990	0.49	0/1336
3	Q	0.36	0/990	0.52	0/1336
3	R	0.37	0/990	0.48	0/1336
3	S	0.35	0/990	0.50	0/1336
3	T	0.38	0/990	0.50	0/1336
3	U	0.35	0/990	0.50	0/1336
3	V	0.37	0/990	0.48	0/1336
3	W	0.35	0/990	0.50	0/1336
4	a	0.38	0/1001	0.48	0/1347
4	b	0.36	0/1001	0.46	0/1347
4	c	0.38	0/1001	0.48	0/1347
4	d	0.37	0/1001	0.46	0/1347
4	e	0.37	0/1001	0.48	0/1347
4	f	0.38	0/1001	0.46	0/1347
4	g	0.37	0/1001	0.46	0/1347
4	h	0.37	0/1001	0.45	0/1347
4	i	0.37	0/1001	0.46	0/1347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	j	0.38	0/1001	0.46	0/1347
4	k	0.38	0/1001	0.46	0/1347
4	l	0.38	0/1001	0.46	0/1347
4	m	0.38	0/1001	0.45	0/1347
4	n	0.38	0/1001	0.46	0/1347
4	o	0.38	0/1001	0.47	0/1347
4	p	0.37	0/1001	0.47	0/1347
4	q	0.38	0/1001	0.46	0/1347
4	r	0.36	0/1001	0.47	0/1347
4	s	0.37	0/1001	0.47	0/1347
4	t	0.35	0/1001	0.46	0/1347
4	u	0.37	0/1001	0.46	0/1347
4	v	0.35	0/1001	0.46	0/1347
4	w	0.36	0/1001	0.47	0/1347
All	All	0.60	0/60649	0.78	127/84634 (0.2%)

There are no bond length outliers.

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	225	DA	O4'-C4'-C3'	-7.25	101.60	104.50
1	1	247	DA	O4'-C4'-C3'	-7.22	101.61	104.50
2	2	487	DA	O4'-C4'-C3'	-6.84	101.76	104.50
2	2	391	DA	O4'-C4'-C3'	-6.83	101.77	104.50
1	1	82	DT	O4'-C4'-C3'	-6.62	101.85	104.50
1	1	106	DT	O4'-C4'-C3'	-6.54	101.88	104.50
2	2	393	DA	O4'-C4'-C3'	-6.41	101.94	104.50
2	2	427	DA	O4'-C4'-C3'	-6.34	101.96	104.50
2	2	370	DT	O4'-C4'-C3'	-6.27	101.99	104.50
2	2	417	DA	O4'-C4'-C3'	-6.19	102.02	104.50
2	2	406	DT	O4'-C4'-C3'	-6.15	102.04	104.50
1	1	211	DA	O4'-C4'-C3'	-6.12	102.05	104.50
2	2	405	DA	O4'-C4'-C3'	-6.10	102.06	104.50
1	1	120	DT	O4'-C4'-C3'	-6.08	102.07	104.50
1	1	30	DT	O4'-C4'-C3'	-6.00	102.10	104.50
2	2	243	DA	O4'-C1'-N9	5.98	112.18	108.00
2	2	401	DA	O4'-C4'-C3'	-5.98	102.11	104.50
2	2	245	DA	O4'-C4'-C3'	-5.95	102.12	104.50
2	2	501	DA	O4'-C4'-C3'	-5.95	102.12	104.50
2	2	244	DT	O4'-C4'-C3'	-5.92	102.13	104.50
2	2	437	DA	O4'-C4'-C3'	-5.92	102.13	104.50
1	1	258	DT	O4'-C4'-C3'	-5.86	102.16	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	46	DT	O4'-C4'-C3'	-5.85	102.16	104.50
2	2	389	DA	O4'-C4'-C3'	-5.84	102.16	104.50
1	1	214	DT	O4'-C4'-C3'	-5.84	102.17	104.50
1	1	274	DT	O4'-C4'-C3'	-5.84	102.17	104.50
2	2	524	DT	O4'-C4'-C3'	-5.83	102.17	104.50
1	1	94	DT	O4'-C4'-C3'	-5.83	102.17	104.50
1	1	118	DT	O4'-C4'-C3'	-5.82	102.17	104.50
2	2	394	DT	O4'-C4'-C3'	-5.81	102.17	104.50
2	2	316	DT	O4'-C4'-C3'	-5.81	102.17	104.50
2	2	377	DA	O4'-C4'-C3'	-5.80	102.18	104.50
2	2	274	DT	O4'-C4'-C3'	-5.79	102.18	104.50
2	2	512	DT	O4'-C4'-C3'	-5.76	102.20	104.50
2	2	510	DT	O4'-C4'-C3'	-5.75	102.20	104.50
2	2	221	DA	O4'-C4'-C3'	-5.73	102.21	104.50
1	1	283	DA	O4'-C4'-C3'	-5.73	102.21	104.50
2	2	238	DT	O4'-C4'-C3'	-5.72	102.21	104.50
1	1	166	DT	O4'-C4'-C3'	-5.72	102.21	104.50
1	1	142	DT	O4'-C4'-C3'	-5.72	102.21	104.50
2	2	382	DT	O4'-C4'-C3'	-5.72	102.21	104.50
2	2	345	DA	O4'-C4'-C3'	-5.70	102.22	104.50
1	1	262	DT	O4'-C4'-C3'	-5.69	102.22	104.50
2	2	474	DT	O4'-C4'-C3'	-5.67	102.23	104.50
2	2	522	DT	O4'-C4'-C3'	-5.66	102.24	104.50
2	2	334	DT	O4'-C4'-C3'	-5.66	102.24	104.50
1	1	250	DT	O4'-C4'-C3'	-5.62	102.25	104.50
2	2	224	DT	O4'-C4'-C3'	-5.61	102.25	104.50
2	2	421	DA	O4'-C1'-N9	5.60	111.92	108.00
1	1	212	DT	O4'-C4'-C3'	-5.60	102.26	104.50
1	1	70	DT	O4'-C4'-C3'	-5.59	102.26	104.50
2	2	441	DA	O4'-C4'-C3'	-5.59	102.26	104.50
2	2	283	DA	O4'-C4'-C3'	-5.59	102.26	104.50
1	1	259	DA	O4'-C4'-C3'	-5.58	102.27	104.50
2	2	281	DA	O4'-C4'-C3'	-5.58	102.27	104.50
2	2	257	DA	O4'-C4'-C3'	-5.57	102.27	104.50
2	2	472	DT	O4'-C4'-C3'	-5.56	102.28	104.50
2	2	379	DA	O4'-C4'-C3'	-5.56	102.28	104.50
2	2	430	DT	O4'-C4'-C3'	-5.55	102.28	104.50
2	2	439	DA	O4'-C4'-C3'	-5.55	102.28	104.50
2	2	486	DT	O4'-C4'-C3'	-5.53	102.29	104.50
1	1	150	DT	O4'-C4'-C3'	-5.53	102.29	104.50
2	2	529	DA	O4'-C1'-N9	5.52	111.87	108.00
2	2	261	DA	O4'-C4'-C3'	-5.52	102.29	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	271	DA	O4'-C4'-C3'	-5.52	102.29	104.50
2	2	351	DA	O4'-C1'-N9	5.51	111.86	108.00
1	1	286	DT	O4'-C4'-C3'	-5.49	102.30	104.50
2	2	451	DA	O4'-C4'-C3'	-5.49	102.30	104.50
2	2	250	DT	O4'-C4'-C3'	-5.47	102.31	104.50
1	1	-2	DT	O4'-C4'-C3'	-5.47	102.31	104.50
2	2	309	DA	O4'-C4'-C3'	-5.47	102.31	104.50
2	2	212	DT	O4'-C4'-C3'	-5.46	102.32	104.50
2	2	426	DT	O4'-C4'-C3'	-5.46	102.32	104.50
1	1	178	DT	O4'-C4'-C3'	-5.43	102.33	104.50
2	2	489	DA	O4'-C4'-C3'	-5.42	102.33	104.50
2	2	496	DT	O4'-C4'-C3'	-5.42	102.33	104.50
1	1	154	DT	O4'-C4'-C3'	-5.42	102.33	104.50
1	1	66	DT	O4'-C4'-C3'	-5.40	102.34	104.50
2	2	349	DA	O4'-C1'-N9	5.40	111.78	108.00
2	2	313	DA	O4'-C4'-C3'	-5.39	102.34	104.50
2	2	469	DA	O4'-C4'-C3'	-5.38	102.35	104.50
1	1	224	DT	O4'-C4'-C3'	-5.36	102.36	104.50
2	2	273	DA	O4'-C4'-C3'	-5.35	102.36	104.50
2	2	457	DA	O4'-C1'-N9	5.34	111.74	108.00
2	2	517	DA	O4'-C4'-C3'	-5.33	102.37	104.50
1	1	200	DT	O4'-C4'-C3'	-5.32	102.37	104.50
2	2	340	DT	O4'-C4'-C3'	-5.27	102.39	104.50
2	2	463	DA	O4'-C4'-C3'	-5.26	102.40	104.50
2	2	234	DT	O4'-C4'-C3'	-5.25	102.40	104.50
1	1	-12	DT	O4'-C4'-C3'	-5.25	102.40	104.50
1	1	60	DT	O4'-C4'-C3'	-5.25	102.40	104.50
2	2	466	DT	O4'-C4'-C3'	-5.24	102.40	104.50
2	2	346	DT	O4'-C4'-C3'	-5.24	102.40	104.50
2	2	321	DA	O4'-C4'-C3'	-5.22	102.41	104.50
2	2	357	DA	O4'-C4'-C3'	-5.22	102.41	104.50
1	1	103	DA	O4'-C4'-C3'	-5.21	102.41	104.50
2	2	400	DT	O4'-C4'-C3'	-5.21	102.42	104.50
1	1	151	DA	O4'-C4'-C3'	-5.19	102.42	104.50
2	2	484	DT	O4'-C4'-C3'	-5.19	102.42	104.50
2	2	298	DT	O4'-C4'-C3'	-5.18	102.43	104.50
2	2	513	DA	O4'-C4'-C3'	-5.18	102.43	104.50
1	1	80	DT	O4'-C4'-C3'	-5.16	102.44	104.50
1	1	238	DT	O4'-C4'-C3'	-5.15	102.44	104.50
2	2	233	DA	O4'-C4'-C3'	-5.15	102.44	104.50
2	2	358	DT	O4'-C4'-C3'	-5.15	102.44	104.50
1	1	164	DT	O4'-C4'-C3'	-5.15	102.44	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	488	DT	O4'-C4'-C3'	-5.14	102.44	104.50
1	1	160	DT	O4'-C4'-C3'	-5.14	102.44	104.50
2	2	499	DA	O4'-C4'-C3'	-5.14	102.44	104.50
1	1	96	DT	O4'-C4'-C3'	-5.13	102.45	104.50
1	1	136	DT	O4'-C4'-C3'	-5.13	102.45	104.50
2	2	265	DA	O4'-C4'-C3'	-5.13	102.45	104.50
2	2	344	DT	O4'-C4'-C3'	-5.13	102.45	104.50
2	2	493	DA	O4'-C4'-C3'	-5.13	102.45	104.50
2	2	297	DA	O4'-C4'-C3'	-5.12	102.45	104.50
2	2	222	DT	O4'-C4'-C3'	-5.09	102.46	104.50
1	1	189	DA	O4'-C4'-C3'	-5.09	102.47	104.50
2	2	364	DT	O4'-C4'-C3'	-5.09	102.47	104.50
2	2	525	DA	O4'-C4'-C3'	-5.07	102.47	104.50
1	1	43	DA	O4'-C4'-C3'	-5.06	102.48	104.50
1	1	-5	DA	O4'-C4'-C3'	-5.02	102.49	104.50
2	2	376	DT	O4'-C4'-C3'	-5.02	102.49	104.50
1	1	42	DT	O4'-C4'-C3'	-5.02	102.49	104.50
2	2	459	DA	O4'-C1'-N9	5.02	111.51	108.00
2	2	520	DT	O4'-C4'-C3'	-5.01	102.50	104.50
1	1	225	DA	C4'-C3'-C2'	-5.00	98.60	103.10
2	2	475	DA	O4'-C4'-C3'	-5.00	102.50	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	B	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	C	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	D	117/129 (91%)	114 (97%)	3 (3%)	0	100	100
3	E	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
3	F	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
3	G	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
3	H	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
3	I	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	J	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	K	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
3	L	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	M	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	N	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
3	O	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
3	P	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
3	Q	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
3	R	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	S	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
3	T	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
3	U	117/129 (91%)	114 (97%)	3 (3%)	0	100	100
3	V	117/129 (91%)	113 (97%)	4 (3%)	0	100	100
3	W	117/129 (91%)	114 (97%)	3 (3%)	0	100	100
4	a	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
4	b	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	c	124/145 (86%)	120 (97%)	4 (3%)	0	100	100
4	d	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
4	e	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	f	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
4	g	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	h	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	i	124/145 (86%)	120 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	j	124/145 (86%)	120 (97%)	4 (3%)	0	100	100
4	k	124/145 (86%)	120 (97%)	4 (3%)	0	100	100
4	l	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	m	124/145 (86%)	120 (97%)	4 (3%)	0	100	100
4	n	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
4	o	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
4	p	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
4	q	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	r	124/145 (86%)	120 (97%)	4 (3%)	0	100	100
4	s	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
4	t	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	u	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	v	124/145 (86%)	122 (98%)	2 (2%)	0	100	100
4	w	124/145 (86%)	120 (97%)	4 (3%)	0	100	100
All	All	5543/6302 (88%)	5371 (97%)	172 (3%)	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	
3	A	105/114 (92%)	104 (99%)	1 (1%)	76	88
3	B	105/114 (92%)	104 (99%)	1 (1%)	76	88
3	C	105/114 (92%)	103 (98%)	2 (2%)	57	78
3	D	105/114 (92%)	105 (100%)	0	100	100
3	E	105/114 (92%)	105 (100%)	0	100	100
3	F	105/114 (92%)	105 (100%)	0	100	100
3	G	105/114 (92%)	104 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	105/114 (92%)	105 (100%)	0	100	100
3	I	105/114 (92%)	104 (99%)	1 (1%)	76	88
3	J	105/114 (92%)	105 (100%)	0	100	100
3	K	105/114 (92%)	105 (100%)	0	100	100
3	L	105/114 (92%)	103 (98%)	2 (2%)	57	78
3	M	105/114 (92%)	104 (99%)	1 (1%)	76	88
3	N	105/114 (92%)	104 (99%)	1 (1%)	76	88
3	O	105/114 (92%)	104 (99%)	1 (1%)	76	88
3	P	105/114 (92%)	105 (100%)	0	100	100
3	Q	105/114 (92%)	104 (99%)	1 (1%)	76	88
3	R	105/114 (92%)	104 (99%)	1 (1%)	76	88
3	S	105/114 (92%)	105 (100%)	0	100	100
3	T	105/114 (92%)	103 (98%)	2 (2%)	57	78
3	U	105/114 (92%)	105 (100%)	0	100	100
3	V	105/114 (92%)	105 (100%)	0	100	100
3	W	105/114 (92%)	103 (98%)	2 (2%)	57	78
4	a	97/100 (97%)	97 (100%)	0	100	100
4	b	97/100 (97%)	97 (100%)	0	100	100
4	c	97/100 (97%)	97 (100%)	0	100	100
4	d	97/100 (97%)	97 (100%)	0	100	100
4	e	97/100 (97%)	97 (100%)	0	100	100
4	f	97/100 (97%)	97 (100%)	0	100	100
4	g	97/100 (97%)	96 (99%)	1 (1%)	76	88
4	h	97/100 (97%)	97 (100%)	0	100	100
4	i	97/100 (97%)	97 (100%)	0	100	100
4	j	97/100 (97%)	97 (100%)	0	100	100
4	k	97/100 (97%)	97 (100%)	0	100	100
4	l	97/100 (97%)	97 (100%)	0	100	100
4	m	97/100 (97%)	97 (100%)	0	100	100
4	n	97/100 (97%)	97 (100%)	0	100	100
4	o	97/100 (97%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	p	97/100 (97%)	97 (100%)	0	100 100
4	q	97/100 (97%)	97 (100%)	0	100 100
4	r	97/100 (97%)	97 (100%)	0	100 100
4	s	97/100 (97%)	97 (100%)	0	100 100
4	t	97/100 (97%)	97 (100%)	0	100 100
4	u	97/100 (97%)	97 (100%)	0	100 100
4	v	97/100 (97%)	97 (100%)	0	100 100
4	w	97/100 (97%)	97 (100%)	0	100 100
All	All	4646/4922 (94%)	4628 (100%)	18 (0%)	91 95

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	92	GLN
3	B	24	LYS
3	C	38	ARG
3	C	75	ASN
3	G	75	ASN
3	I	75	ASN
3	L	38	ARG
3	L	92	GLN
3	M	75	ASN
3	N	92	GLN
3	O	24	LYS
3	Q	24	LYS
3	R	92	GLN
3	T	75	ASN
3	T	98	ARG
3	W	75	ASN
3	W	92	GLN
4	g	55	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	18	HIS
3	A	65	ASN
3	B	18	HIS

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Mol	Chain	Res	Type
3	B	65	ASN
3	B	114	ASN
3	C	116	GLN
3	D	65	ASN
3	D	114	ASN
3	E	18	HIS
3	F	18	HIS
3	F	114	ASN
3	G	65	ASN
3	G	114	ASN
3	H	18	HIS
3	H	65	ASN
3	I	18	HIS
3	I	65	ASN
3	I	114	ASN
3	J	18	HIS
3	J	56	GLN
3	J	65	ASN
3	J	75	ASN
3	J	114	ASN
3	K	18	HIS
3	K	65	ASN
3	L	18	HIS
3	L	56	GLN
3	L	75	ASN
3	L	110	GLN
3	L	114	ASN
3	L	116	GLN
3	M	18	HIS
3	M	65	ASN
3	M	114	ASN
3	N	18	HIS
3	N	114	ASN
3	O	18	HIS
3	O	65	ASN
3	P	18	HIS
3	P	56	GLN
3	P	65	ASN
3	P	75	ASN
3	P	114	ASN
3	Q	18	HIS
3	Q	65	ASN

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Mol	Chain	Res	Type
3	Q	114	ASN
3	Q	116	GLN
3	R	18	HIS
3	R	56	GLN
3	R	75	ASN
3	R	114	ASN
3	S	18	HIS
3	S	114	ASN
3	T	18	HIS
3	T	75	ASN
3	T	114	ASN
3	U	18	HIS
3	V	18	HIS
3	V	65	ASN
3	V	114	ASN
3	W	18	HIS
3	W	56	GLN
3	W	65	ASN
4	g	98	GLN
4	v	98	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.

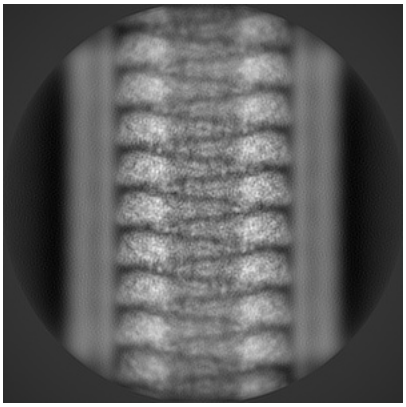
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21094. These allow visual inspection of the internal detail of the map and identification of artifacts.

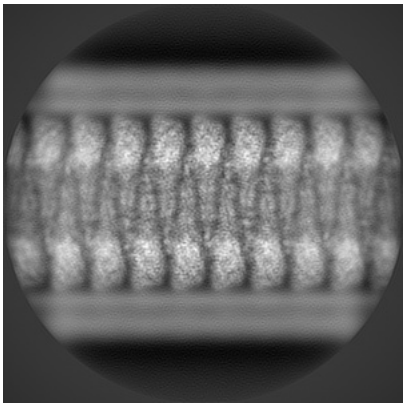
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

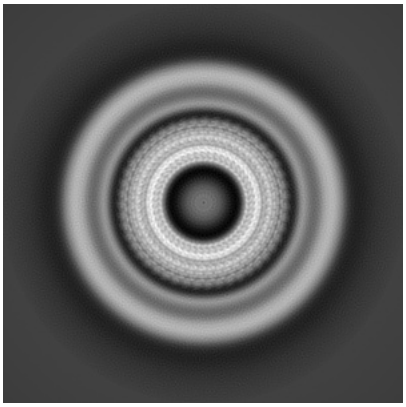
6.1.1 Primary map



X



Y

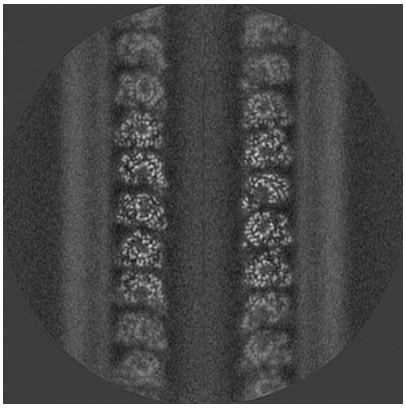


Z

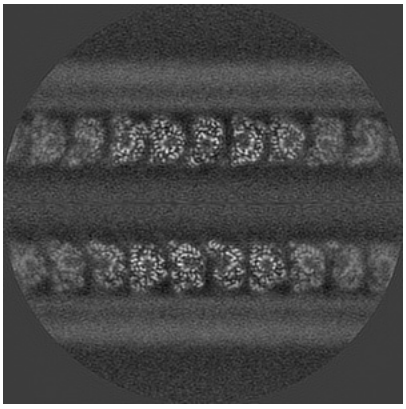
The images above show the map projected in three orthogonal directions.

6.2 Central slices

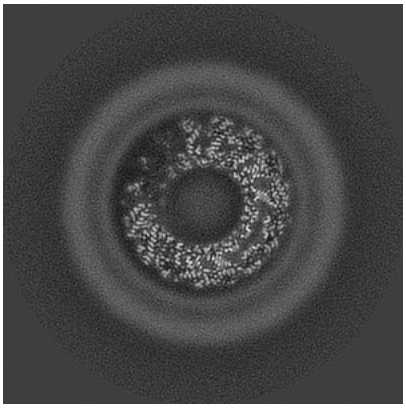
6.2.1 Primary map



X Index: 160



Y Index: 160

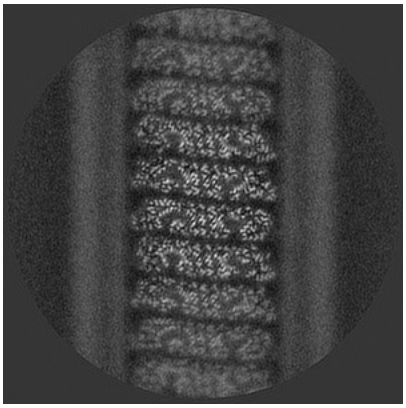


Z Index: 160

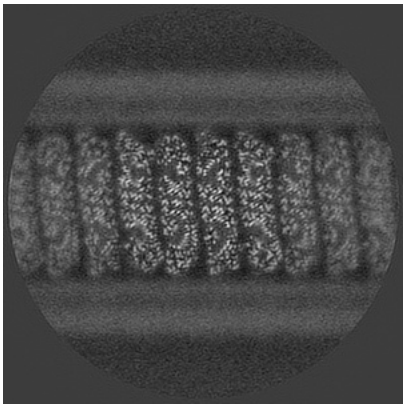
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

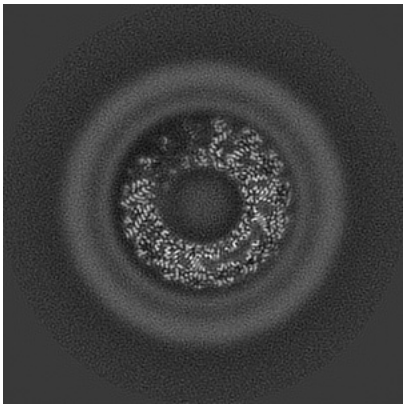
6.3.1 Primary map



X Index: 119



Y Index: 201

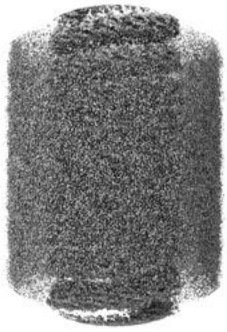


Z Index: 158

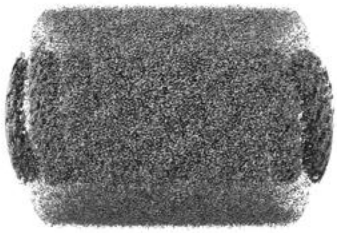
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

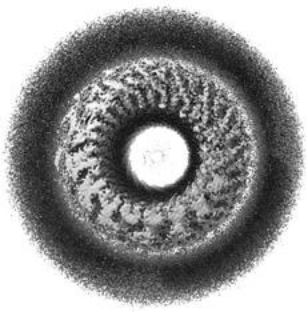
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

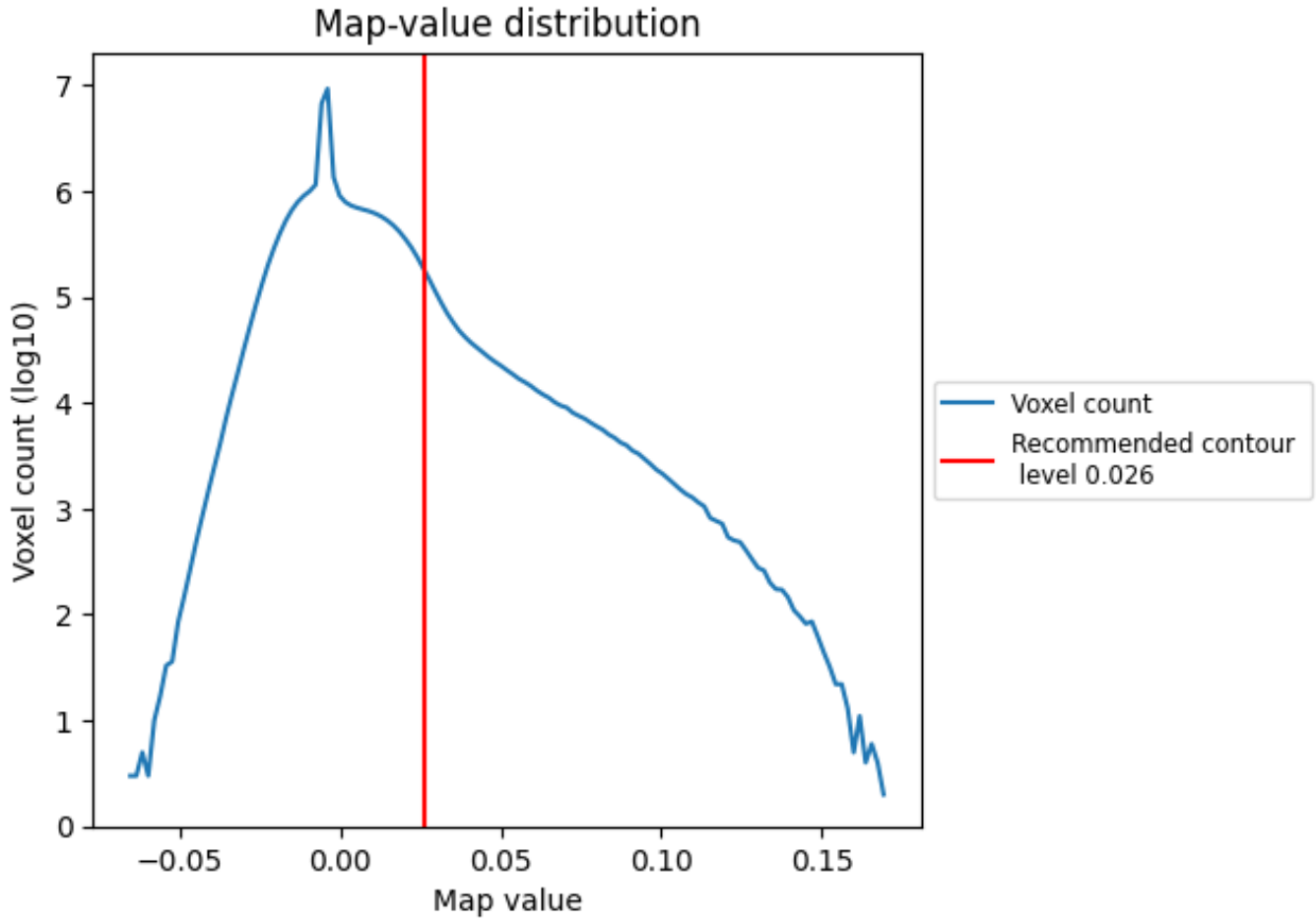
6.5 Mask visualisation (i)

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

7 Map analysis

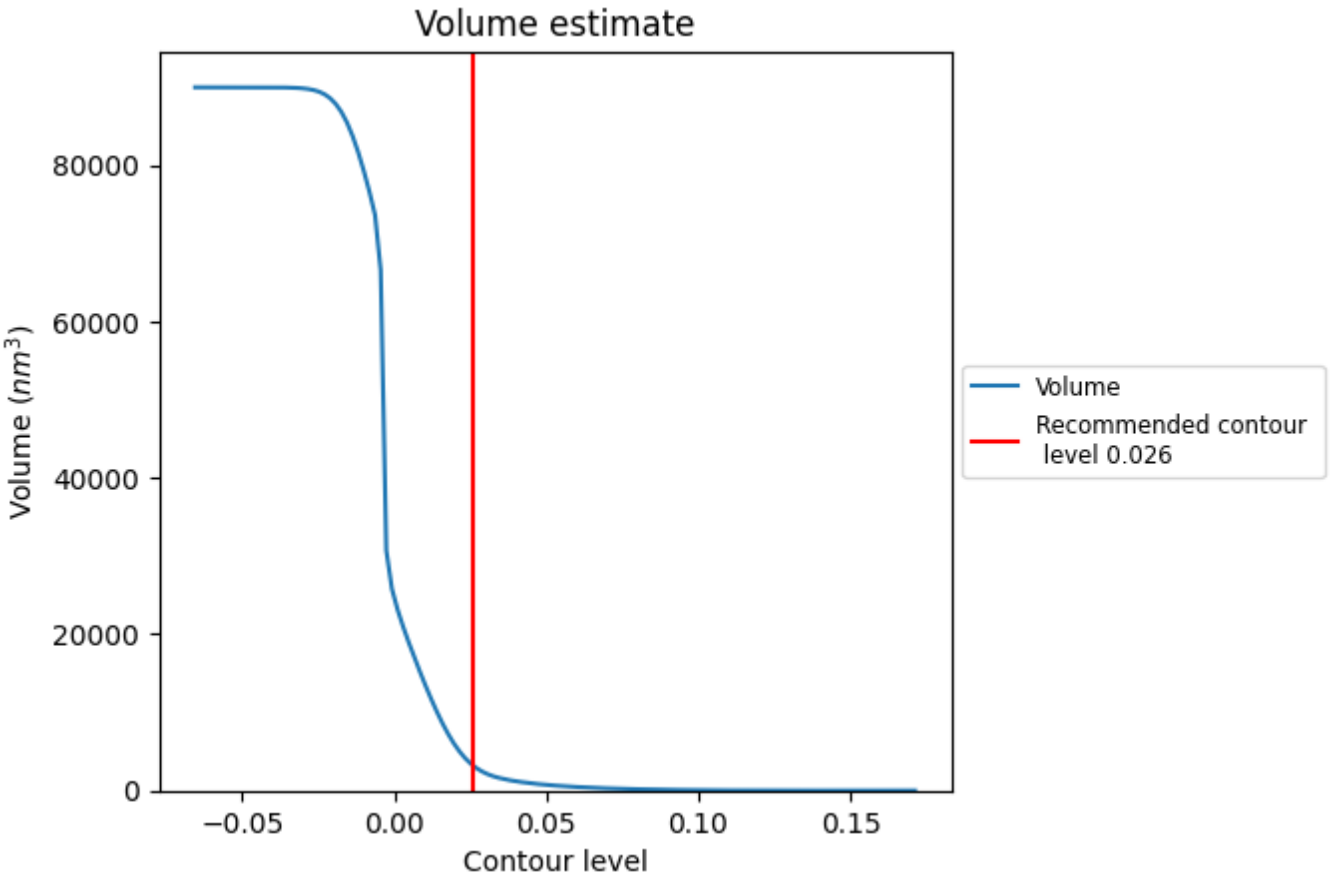
This section contains the results of statistical analysis of the map.

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.

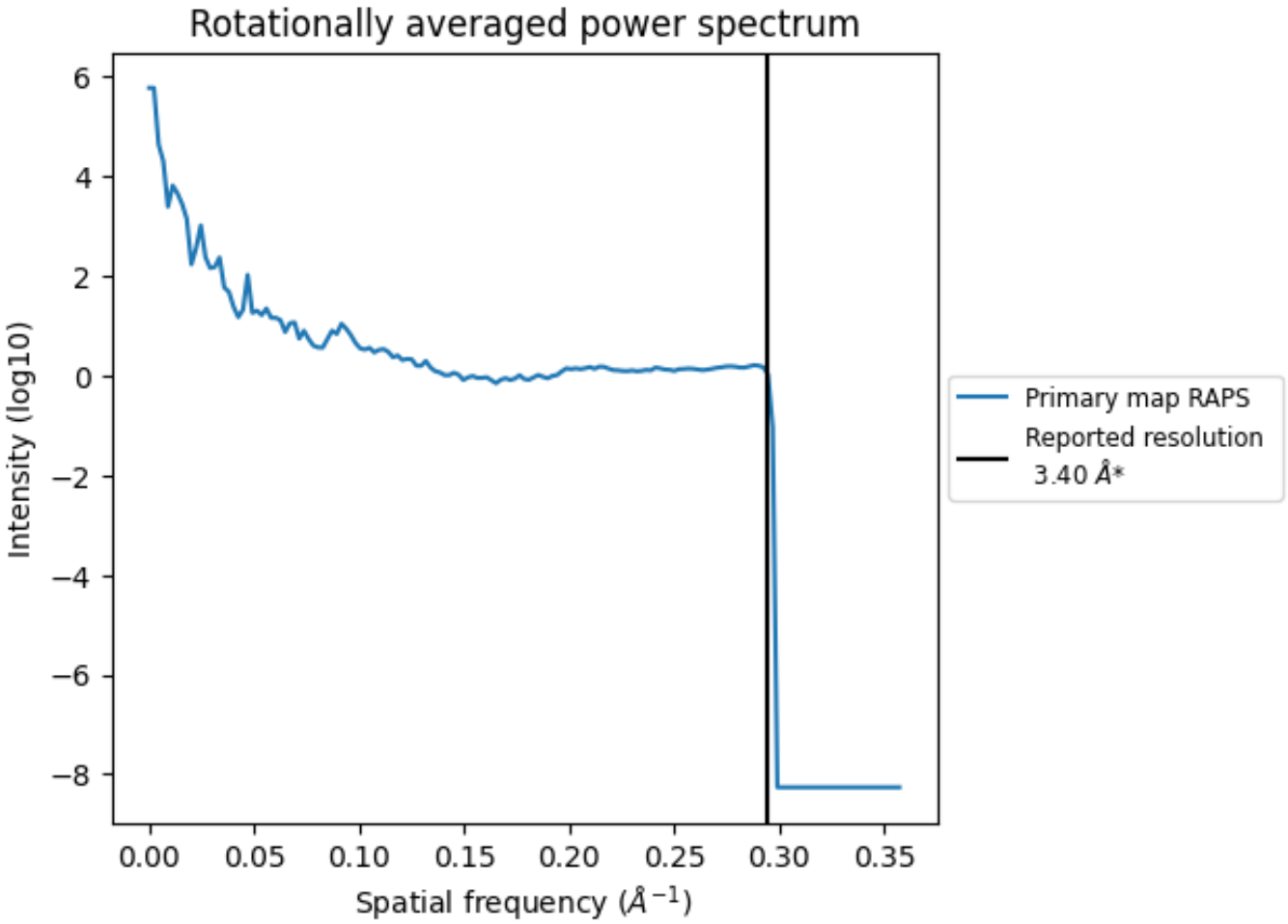
7.2 Volume estimate



The volume at the recommended contour level is 3192 nm^3; this corresponds to an approximate mass of 2884 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 0.294 Å^{-1}

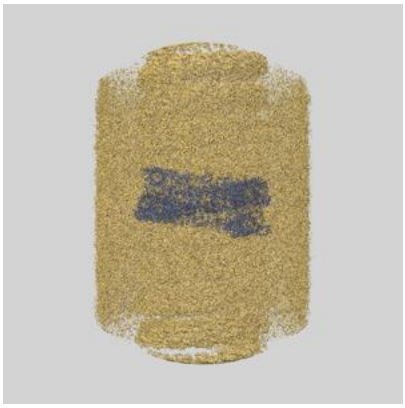
8 Fourier-Shell correlation (i)

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

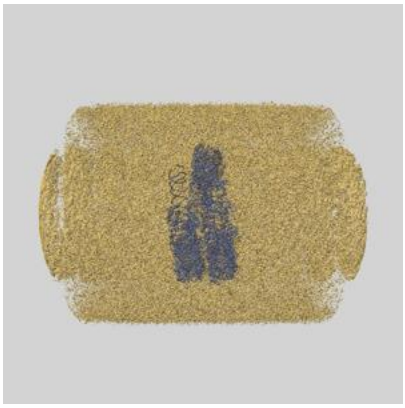
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21094 and PDB model 6V7B. Per-residue inclusion information can be found in section 3 on page 11.

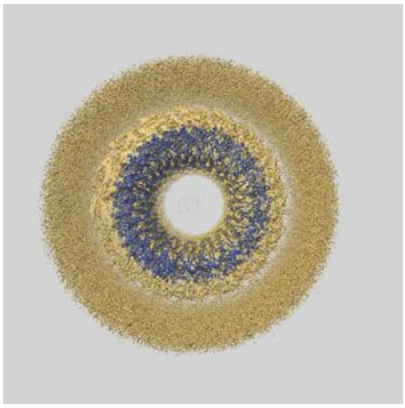
9.1 Map-model overlay



X



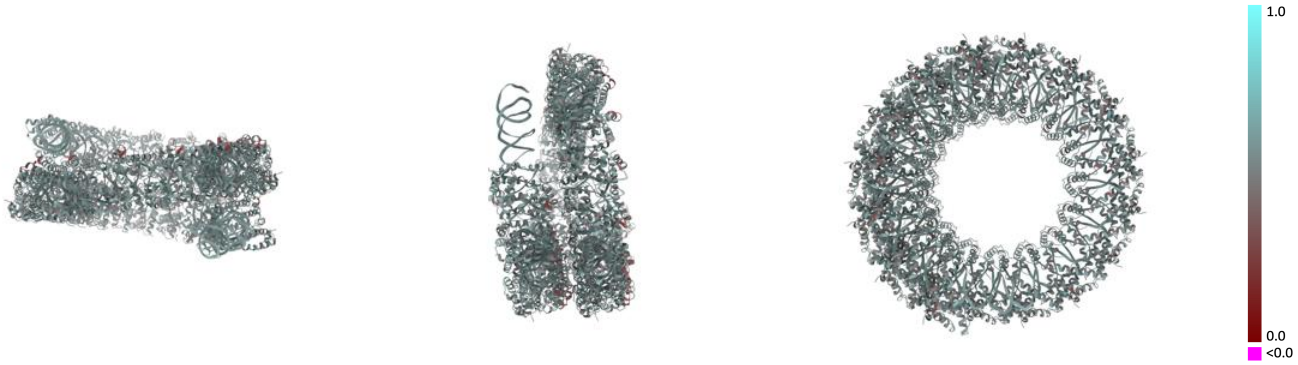
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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.

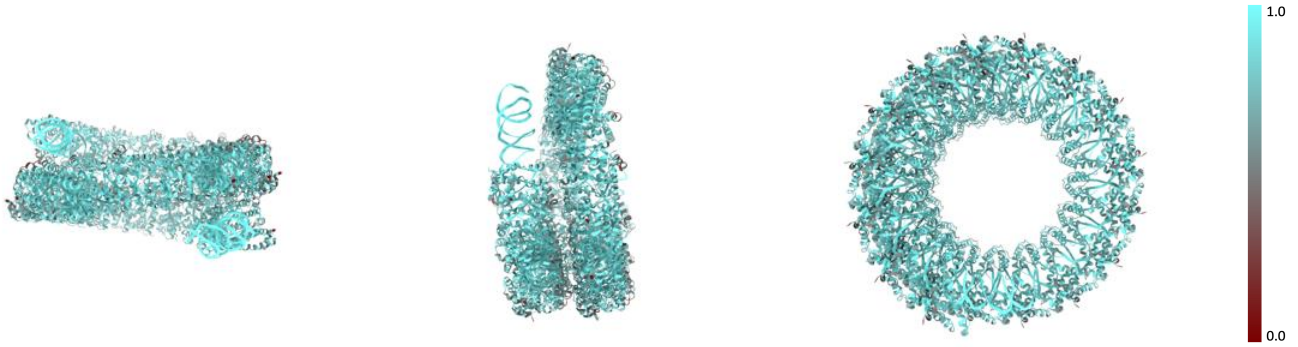
9.2 Q-score mapped to coordinate model (i)



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.

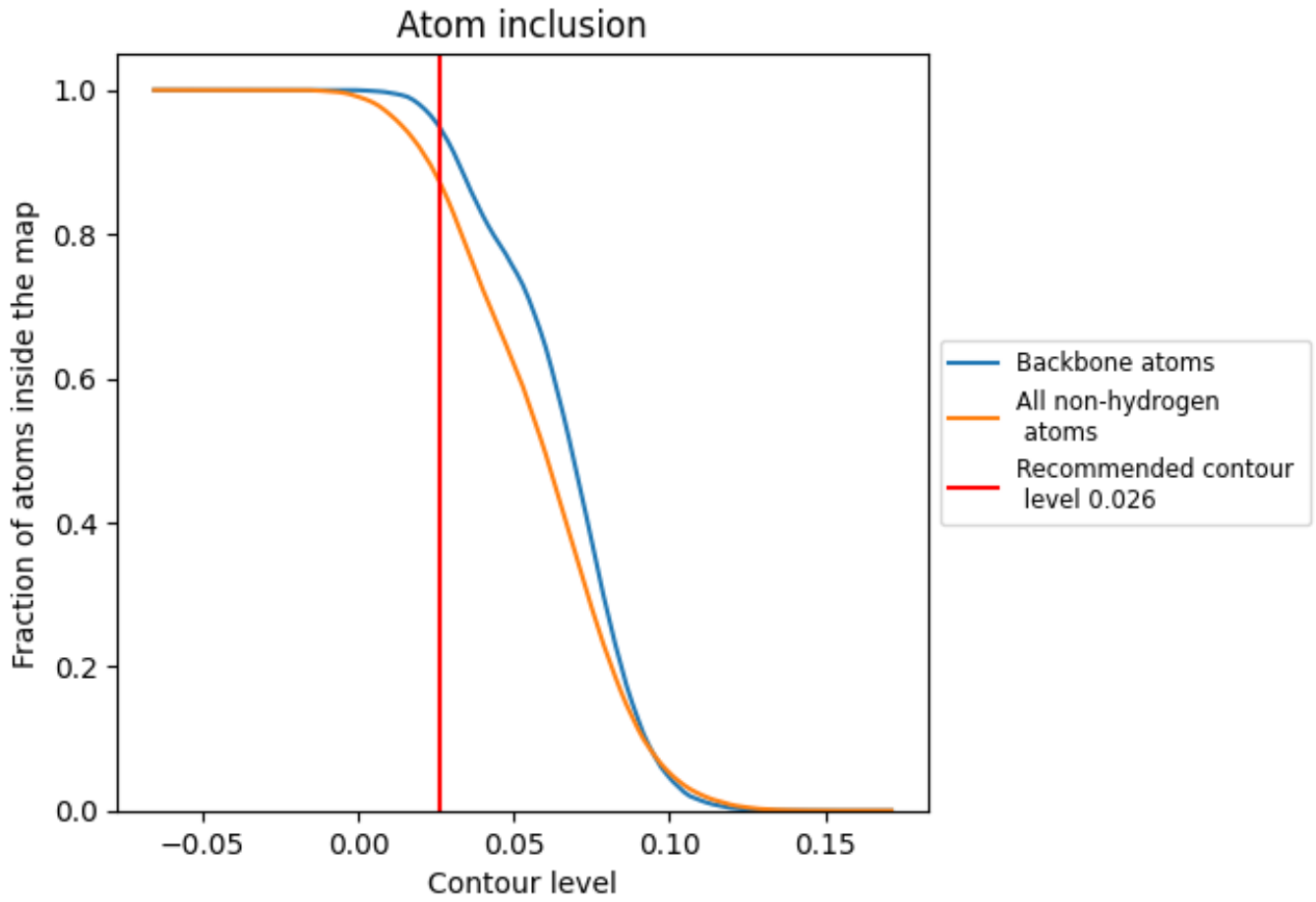
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8739	0.5380
1	0.9991	0.5690
2	0.9921	0.5560
A	0.8358	0.5230
B	0.8453	0.5230
C	0.8294	0.5200
D	0.8347	0.5290
E	0.8443	0.5200
F	0.8347	0.5240
G	0.8379	0.5210
H	0.8549	0.5270
I	0.8358	0.5240
J	0.8400	0.5210
K	0.8411	0.5210
L	0.8358	0.5210
M	0.8316	0.5240
N	0.8390	0.5250
O	0.8422	0.5250
P	0.8199	0.5270
Q	0.8400	0.5200
R	0.8337	0.5190
S	0.8273	0.5210
T	0.8294	0.5230
U	0.8242	0.5230
V	0.8284	0.5190
W	0.8347	0.5230
a	0.8384	0.5390
b	0.8520	0.5420
c	0.8426	0.5400
d	0.8405	0.5390
e	0.8510	0.5370
f	0.8426	0.5400
g	0.8478	0.5400
h	0.8437	0.5400
i	0.8342	0.5390

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Chain	Atom inclusion	Q-score
j	0.8416	0.5420
k	0.8342	0.5330
l	0.8300	0.5370
m	0.8426	0.5430
n	0.8311	0.5380
o	0.8353	0.5360
p	0.8321	0.5370
q	0.8332	0.5370
r	0.8426	0.5410
s	0.8363	0.5380
t	0.8332	0.5400
u	0.8321	0.5340
v	0.8374	0.5410
w	0.8269	0.5330