



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 05:10 PM UTC

PDB ID : 8UK2 / pdb_00008uk2
EMDB ID : EMD-42343
Title : The rotavirus VP5*/VP8* conformational transition permeabilizes membranes to Ca²⁺ (class 5 reconstruction)
Authors : De Sautu, M.; Herrmann, T.; Jenni, S.; Harrison, S.C.
Deposited on : 2023-10-12
Resolution : 8.00 Å(reported)
Based on initial model : 6WXG

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:

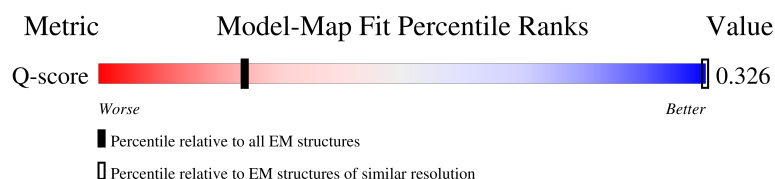
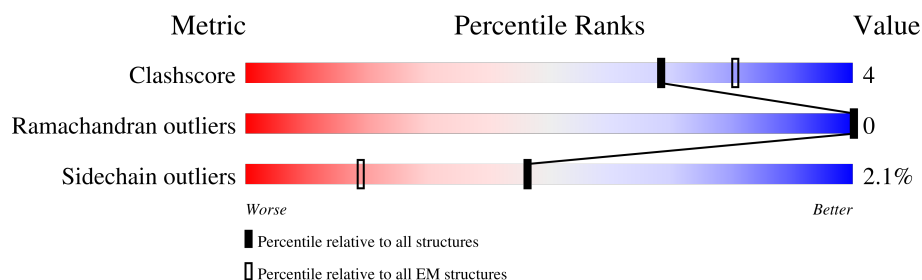
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 8.00 Å.

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



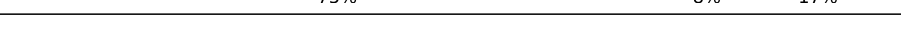
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

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

Mol	Chain	Length	Quality of chain
1	1	776	6% 31% 65%
1	2	776	7% 32% 65%
1	3	776	10% 31% 65%
2	a	326	69% 10% 21%

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Mol	Chain	Length	Quality of chain
2	b	326	
2	c	326	
2	d	326	
2	e	326	
2	f	326	
2	g	326	
2	h	326	
2	i	326	
2	j	326	
2	k	326	
2	l	326	
2	m	326	
2	n	326	
2	o	326	
2	p	326	
2	q	326	
2	r	326	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 88254 atoms, of which 43479 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 Outer capsid protein VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		
1	2	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		
1	3	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		

- Molecule 2 is a protein called Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	f	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
2	g	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	h	259	Total	C	H	N	O	S	0	0
			4041	1298	1994	324	409	16		
2	i	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	j	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	k	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
2	l	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
2	m	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	n	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
2	o	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
2	p	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	q	259	Total	C	H	N	O	S	0	0
			4041	1298	1994	324	409	16		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	r	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	a	259	Total	C	H	N	O	S	0	0
			4041	1298	1994	324	409	16		
2	b	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	c	261	Total	C	H	N	O	S	0	0
			4074	1308	2011	327	412	16		
2	d	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
2	e	260	Total	C	H	N	O	S	0	0
			4050	1302	1998	323	411	16		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
3	f	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	g	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	h	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	i	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	j	1	Total	C	H	N	O	0
			28	8	14	1	5	

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Mol	Chain	Residues	Atoms					AltConf
3	k	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	l	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	m	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	n	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	o	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	p	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	q	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	r	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	a	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	b	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	c	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	d	1	Total	C	H	N	O	0
			28	8	14	1	5	
3	e	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	f	3	Total	Ca	0
			3	3	
4	g	3	Total	Ca	0
			3	3	
4	h	3	Total	Ca	0
			3	3	
4	i	3	Total	Ca	0
			3	3	
4	j	3	Total	Ca	0
			3	3	
4	k	3	Total	Ca	0
			3	3	

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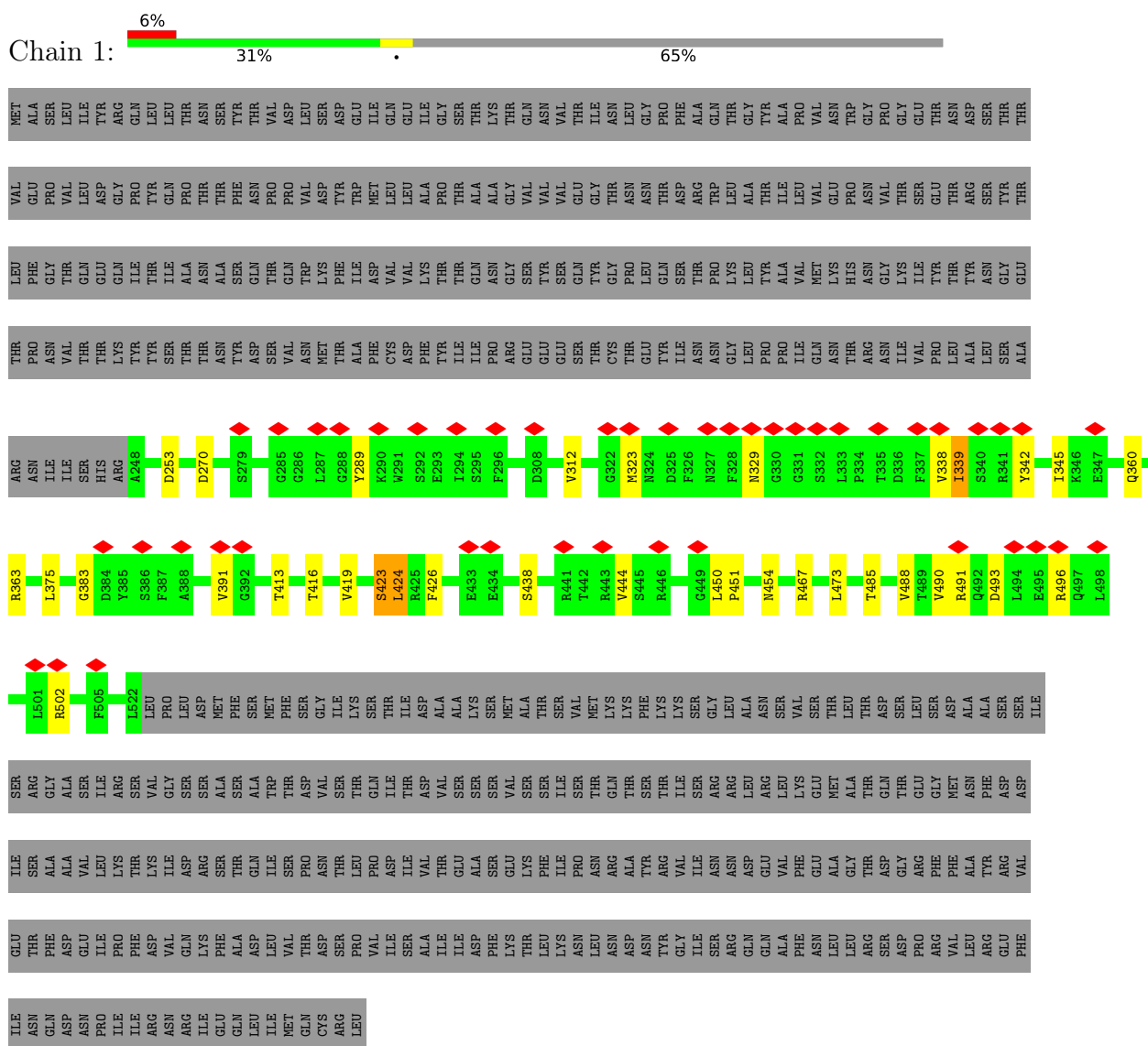
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Mol	Chain	Residues	Atoms		AltConf
4	l	3	Total 3	Ca 3	0
4	m	3	Total 3	Ca 3	0
4	n	3	Total 3	Ca 3	0
4	o	3	Total 3	Ca 3	0
4	p	3	Total 3	Ca 3	0
4	q	3	Total 3	Ca 3	0
4	r	3	Total 3	Ca 3	0
4	a	3	Total 3	Ca 3	0
4	b	3	Total 3	Ca 3	0
4	c	3	Total 3	Ca 3	0
4	d	3	Total 3	Ca 3	0
4	e	3	Total 3	Ca 3	0

3 Residue-property plots

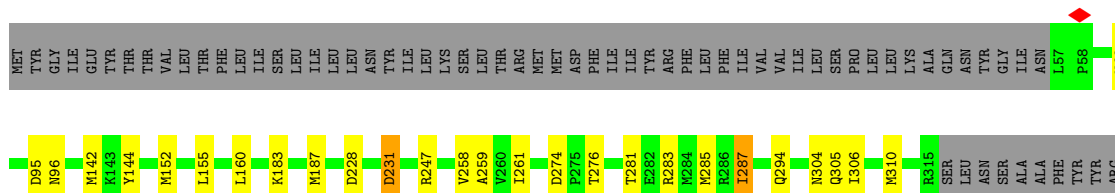
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Outer capsid protein VP4



• Molecule 1: Outer capsid protein VP4





ILE

- Molecule 2: Outer capsid glycoprotein VP7

Chain i:  74% 9% 17%

MET	TRR	I60	L81	I81	GLU	THR	THR	THR	VAL	THR	THR	PHE	LEU	ILE	SER	LEU	ILE	LEU	ASN	TYR	ILE	ILE	LYS	SER	LEU	THR	MET	ASP	PHE	ILE	ILE	TYR	ARG	PHE	LEU	PHE	ILE	VAL	VAL	ILE	SER	PRO	LEU	LEU	LYS	ALA	GLN	ASN	TYR	GLY	I55	N69	T75
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

S79	I60	L81	T87	W111	Y121	T122	D123	I124	I124	L141	L160	Q176	K183	S186	M187	E216	D228	D231	R247	I271	T272	A273	P275	P276	T277	T281	E282	R283	I307	S316	L317	Y324	R325	I326
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- Molecule 2: Outer capsid glycoprotein VP7

Chain j:  73% 10% 17%

MET	TRR	GLY	ILE	GLU	TYR	THR	THR	VAL	THR	THR	PHE	LEU	ILE	SER	LEU	ILE	LEU	ASN	TYR	ILE	ILE	LYS	SER	LEU	THR	ARG	MET	ASP	PHE	ILE	ILE	TYR	ARG	PHE	LEU	PHE	ILE	VAL	VAL	ILE	SER	PRO	LEU	LEU	LYS	ALA	GLN	ASN	TYR	GLY	I55	E74	T78
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Y121	T122	D123	I124	A125	D130	F131	Q132	N138	L141	L160	Q176	K183	W184	I185	D211	T214	F215	E216	A219	K223	L224	V225	D228	V258	A259	V260	T277	T281	E282	R283	M284	M285	R286	Q294	I306	R313	S316	I326
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- Molecule 2: Outer capsid glycoprotein VP7

Chain k:  73% 8% 19%

MET	TRR	GLY	ILE	GLU	TYR	THR	THR	VAL	THR	THR	PHE	LEU	ILE	SER	LEU	ILE	LEU	ASN	TYR	ILE	ILE	LYS	SER	LEU	THR	ARG	MET	ASP	PHE	ILE	ILE	TYR	ARG	PHE	LEU	PHE	ILE	VAL	VAL	ILE	LEU	SER	PRO	LEU	LEU	LYS	ALA	Q51	N52	T60	N69	E74	T75
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S79	W111	M142	D145	A146	T147	Q149	L155	L160	Y175	K183	L208	E216	D228	T261	V268	I271	T281	E282	M284	I287	Q294	I307	R315	SER	LEU	ASN	SER	ALA	ALA	PHE	TYR	TYR	ARG	ILE
-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 2: Outer capsid glycoprotein VP7

Chain l:  71% 10% 19%

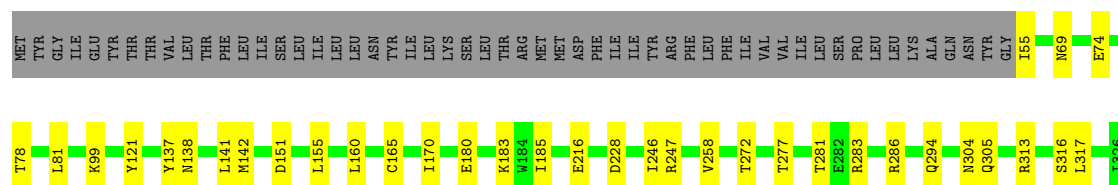
MET	TRR	GLY	GLU	TYR	THR	THR	VAL	THR	THR	PHE	LEU	ILE	SER	LEU	ILE	LEU	ASN	TYR	ILE	ILE	LYS	SER	LEU	THR	ARG	MET	ASP	PHE	ILE	ILE	TYR	ARG	PHE	LEU	PHE	ILE	VAL	VAL	ILE	LEU	SER	PRO	LEU	LEU	LYS	ALA	ALA	Q51	D123	I124	N138	M142	K143	Y144
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M152	L155	L158	L159	L160	M161	E162	D169	I170	T171	L172	S186	M187	T202	T209	E216	V225	D228	I246	V258	A259	V260	V268	D274	F275	T276	T281	E282	R283	M285	R286	Q294	I306	R315	SER	LEU	ASN	SER	ALA	ALA	PHE
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

TYR
TYR
ARG
ILE

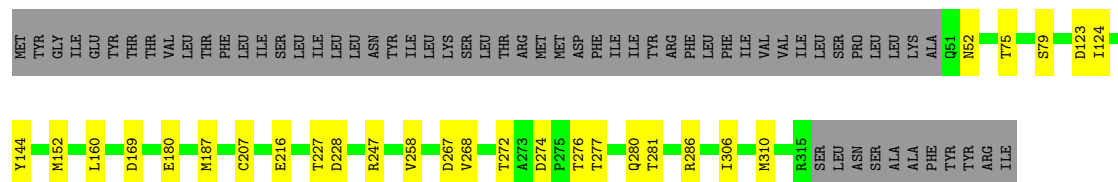
- Molecule 2: Outer capsid glycoprotein VP7

Chain m:  73% 11% 17%



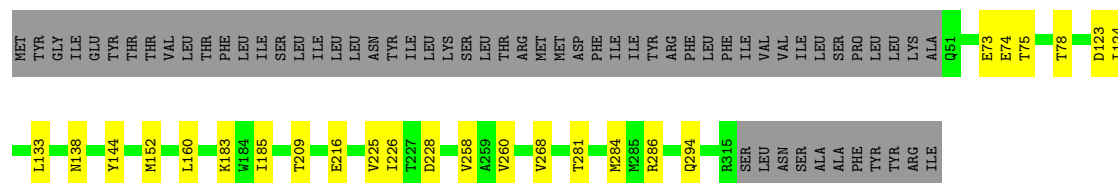
• Molecule 2: Outer capsid glycoprotein VP7

Chain n: 73% 9% 19%



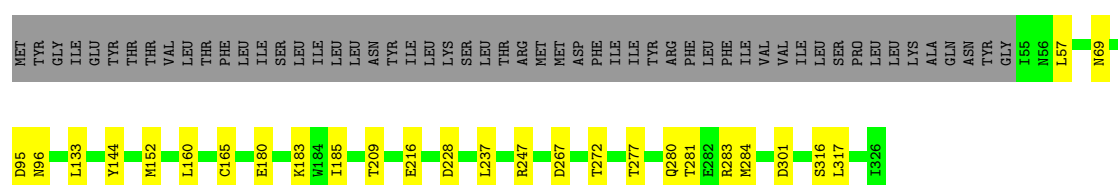
• Molecule 2: Outer capsid glycoprotein VP7

Chain o: 74% 8% 19%



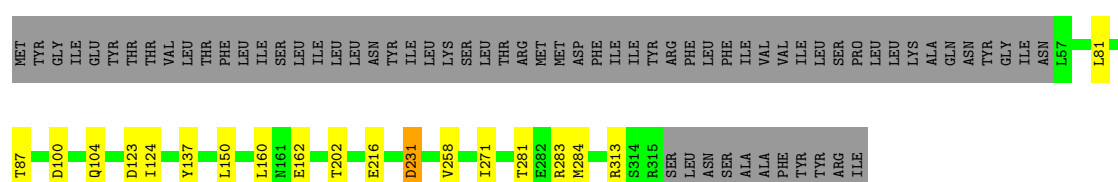
• Molecule 2: Outer capsid glycoprotein VP7

Chain p: 75% 8% 17%



• Molecule 2: Outer capsid glycoprotein VP7

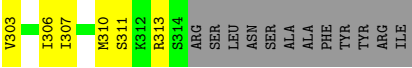
Chain q: 74% 6% 21%



• Molecule 2: Outer capsid glycoprotein VP7



- Molecule 2: Outer capsid glycoprotein VP7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56593	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.027	Depositor
Minimum map value	-0.012	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/2232	0.40	0/3032
1	2	0.20	0/2232	0.41	0/3032
1	3	0.21	0/2232	0.42	0/3032
2	a	0.19	0/2089	0.43	0/2854
2	b	0.19	0/2200	0.44	0/3005
2	c	0.19	0/2105	0.44	0/2876
2	d	0.20	0/2139	0.44	0/2922
2	e	0.20	0/2094	0.45	0/2862
2	f	0.19	0/2139	0.43	0/2922
2	g	0.19	0/2200	0.45	0/3005
2	h	0.19	0/2089	0.43	0/2854
2	i	0.20	0/2200	0.44	0/3005
2	j	0.20	0/2200	0.45	0/3005
2	k	0.19	0/2139	0.45	0/2922
2	l	0.19	0/2139	0.44	0/2922
2	m	0.20	0/2200	0.45	0/3005
2	n	0.19	0/2139	0.43	0/2922
2	o	0.19	0/2139	0.44	0/2922
2	p	0.19	0/2200	0.44	0/3005
2	q	0.19	0/2089	0.43	0/2854
2	r	0.18	0/2200	0.44	0/3005
All	All	0.19	0/45396	0.44	0/61963

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	e	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	e	311	SER	Peptide

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	1	2184	2107	2107	22	0
1	2	2184	2107	2107	14	0
1	3	2184	2107	2107	21	0
2	a	2047	1994	1993	20	0
2	b	2155	2099	2099	26	0
2	c	2063	2011	2010	17	0
2	d	2096	2037	2036	14	0
2	e	2052	1998	1997	21	0
2	f	2096	2037	2036	20	0
2	g	2155	2099	2098	15	0
2	h	2047	1994	1993	16	0
2	i	2155	2099	2098	15	0
2	j	2155	2099	2098	17	0
2	k	2096	2037	2036	15	0
2	l	2096	2037	2036	21	0
2	m	2155	2099	2098	23	0
2	n	2096	2037	2036	17	0
2	o	2096	2037	2036	14	0
2	p	2155	2099	2098	14	0
2	q	2047	1994	1993	11	0
2	r	2155	2099	2098	17	0
3	a	14	14	13	1	0
3	b	14	14	13	0	0
3	c	14	14	13	1	0
3	d	14	14	13	0	0
3	e	14	14	13	0	0
3	f	14	14	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	g	14	14	13	0	0
3	h	14	14	13	1	0
3	i	14	14	13	1	0
3	j	14	14	13	0	0
3	k	14	14	13	1	0
3	l	14	14	13	0	0
3	m	14	14	13	1	0
3	n	14	14	13	0	0
3	o	14	14	13	0	0
3	p	14	14	13	1	0
3	q	14	14	13	0	0
3	r	14	14	13	1	0
4	a	3	0	0	0	0
4	b	3	0	0	0	0
4	c	3	0	0	0	0
4	d	3	0	0	0	0
4	e	3	0	0	0	0
4	f	3	0	0	0	0
4	g	3	0	0	0	0
4	h	3	0	0	0	0
4	i	3	0	0	0	0
4	j	3	0	0	0	0
4	k	3	0	0	0	0
4	l	3	0	0	0	0
4	m	3	0	0	0	0
4	n	3	0	0	0	0
4	o	3	0	0	0	0
4	p	3	0	0	0	0
4	q	3	0	0	0	0
4	r	3	0	0	0	0
All	All	44775	43479	43444	325	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 4.

The worst 5 of 325 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)
1:1:485:THR:HG1	1:2:412:SER:HG	1.26	0.80
2:b:160:LEU:O	2:b:283:ARG:NH2	2.22	0.72
1:3:270:ASP:OD1	1:3:467:ARG:NH1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:160:LEU:O	2:k:283:ARG:NH2	2.23	0.71
2:f:142:MET:HE2	2:f:155:LEU:HD23	1.70	0.71

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	1	273/776 (35%)	273 (100%)	0	0	100	100
1	2	273/776 (35%)	273 (100%)	0	0	100	100
1	3	273/776 (35%)	273 (100%)	0	0	100	100
2	a	257/326 (79%)	257 (100%)	0	0	100	100
2	b	270/326 (83%)	269 (100%)	1 (0%)	0	100	100
2	c	259/326 (79%)	258 (100%)	1 (0%)	0	100	100
2	d	263/326 (81%)	263 (100%)	0	0	100	100
2	e	258/326 (79%)	257 (100%)	1 (0%)	0	100	100
2	f	263/326 (81%)	263 (100%)	0	0	100	100
2	g	270/326 (83%)	269 (100%)	1 (0%)	0	100	100
2	h	257/326 (79%)	257 (100%)	0	0	100	100
2	i	270/326 (83%)	270 (100%)	0	0	100	100
2	j	270/326 (83%)	268 (99%)	2 (1%)	0	100	100
2	k	263/326 (81%)	263 (100%)	0	0	100	100
2	l	263/326 (81%)	263 (100%)	0	0	100	100
2	m	270/326 (83%)	269 (100%)	1 (0%)	0	100	100
2	n	263/326 (81%)	263 (100%)	0	0	100	100
2	o	263/326 (81%)	263 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	p	270/326 (83%)	270 (100%)	0	0	100	100
2	q	257/326 (79%)	257 (100%)	0	0	100	100
2	r	270/326 (83%)	269 (100%)	1 (0%)	0	100	100
All	All	5575/8196 (68%)	5567 (100%)	8 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	241/688 (35%)	234 (97%)	7 (3%)	37	58
1	2	241/688 (35%)	235 (98%)	6 (2%)	42	63
1	3	241/688 (35%)	232 (96%)	9 (4%)	30	51
2	a	233/295 (79%)	231 (99%)	2 (1%)	70	79
2	b	244/295 (83%)	238 (98%)	6 (2%)	42	63
2	c	235/295 (80%)	232 (99%)	3 (1%)	61	74
2	d	238/295 (81%)	233 (98%)	5 (2%)	47	65
2	e	234/295 (79%)	229 (98%)	5 (2%)	47	65
2	f	238/295 (81%)	234 (98%)	4 (2%)	53	69
2	g	244/295 (83%)	239 (98%)	5 (2%)	48	66
2	h	233/295 (79%)	230 (99%)	3 (1%)	61	74
2	i	244/295 (83%)	239 (98%)	5 (2%)	48	66
2	j	244/295 (83%)	238 (98%)	6 (2%)	42	63
2	k	238/295 (81%)	233 (98%)	5 (2%)	47	65
2	l	238/295 (81%)	230 (97%)	8 (3%)	32	54
2	m	244/295 (83%)	241 (99%)	3 (1%)	63	75
2	n	238/295 (81%)	235 (99%)	3 (1%)	61	74
2	o	238/295 (81%)	231 (97%)	7 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	p	244/295 (83%)	238 (98%)	6 (2%)	42	63
2	q	233/295 (79%)	229 (98%)	4 (2%)	53	69
2	r	244/295 (83%)	239 (98%)	5 (2%)	48	66
All	All	5027/7374 (68%)	4920 (98%)	107 (2%)	46	65

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	l	283	ARG
2	p	133	LEU
2	d	149	GLN
2	m	185	ILE
2	o	74	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	a	288	ASN
2	e	104	GLN
2	c	132	GLN
2	d	149	GLN
2	e	305	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 72 ligands modelled in this entry, 54 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	f	401	2	14,14,15	0.38	0	17,19,21	0.44	0
3	NAG	i	403	2	14,14,15	0.64	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	c	403	2	14,14,15	0.62	1 (7%)	17,19,21	0.72	1 (5%)
3	NAG	e	401	2	14,14,15	0.21	0	17,19,21	0.58	0
3	NAG	n	401	2	14,14,15	0.33	0	17,19,21	0.36	0
3	NAG	m	401	2	14,14,15	0.63	1 (7%)	17,19,21	0.73	1 (5%)
3	NAG	g	401	2	14,14,15	0.45	0	17,19,21	0.46	0
3	NAG	b	401	-	14,14,15	0.24	0	17,19,21	0.51	0
3	NAG	o	403	2	14,14,15	0.50	0	17,19,21	0.47	0
3	NAG	l	403	2	14,14,15	0.41	0	17,19,21	0.48	0
3	NAG	d	404	2	14,14,15	0.39	0	17,19,21	0.40	0
3	NAG	h	401	2	14,14,15	0.63	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	p	401	2	14,14,15	0.55	0	17,19,21	0.76	1 (5%)
3	NAG	q	401	2	14,14,15	0.47	0	17,19,21	0.71	1 (5%)
3	NAG	k	401	2	14,14,15	0.65	1 (7%)	17,19,21	0.80	1 (5%)
3	NAG	j	402	2	14,14,15	0.37	0	17,19,21	0.37	0
3	NAG	r	403	2	14,14,15	0.65	1 (7%)	17,19,21	0.78	1 (5%)
3	NAG	a	401	2	14,14,15	0.67	1 (7%)	17,19,21	0.78	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	f	401	2	-	0/6/23/26	0/1/1/1
3	NAG	i	403	2	-	0/6/23/26	0/1/1/1
3	NAG	c	403	2	-	2/6/23/26	0/1/1/1
3	NAG	e	401	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	n	401	2	-	0/6/23/26	0/1/1/1
3	NAG	m	401	2	-	0/6/23/26	0/1/1/1
3	NAG	g	401	2	-	1/6/23/26	0/1/1/1
3	NAG	b	401	-	-	0/6/23/26	0/1/1/1
3	NAG	o	403	2	-	0/6/23/26	0/1/1/1
3	NAG	l	403	2	-	0/6/23/26	0/1/1/1
3	NAG	d	404	2	-	0/6/23/26	0/1/1/1
3	NAG	h	401	2	-	0/6/23/26	0/1/1/1
3	NAG	p	401	2	-	2/6/23/26	0/1/1/1
3	NAG	q	401	2	-	0/6/23/26	0/1/1/1
3	NAG	k	401	2	-	0/6/23/26	0/1/1/1
3	NAG	j	402	2	-	0/6/23/26	0/1/1/1
3	NAG	r	403	2	-	0/6/23/26	0/1/1/1
3	NAG	a	401	2	-	0/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	401	NAG	C1-C2	2.31	1.55	1.52
3	r	403	NAG	C1-C2	2.25	1.55	1.52
3	k	401	NAG	C1-C2	2.23	1.55	1.52
3	i	403	NAG	C1-C2	2.21	1.55	1.52
3	m	401	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	k	401	NAG	C1-O5-C5	2.86	116.01	112.19
3	r	403	NAG	C1-O5-C5	2.76	115.88	112.19
3	a	401	NAG	C1-O5-C5	2.70	115.81	112.19
3	p	401	NAG	C1-O5-C5	2.61	115.69	112.19
3	i	403	NAG	C1-O5-C5	2.59	115.66	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	c	403	NAG	C4-C5-C6-O6
3	c	403	NAG	O5-C5-C6-O6
3	p	401	NAG	O5-C5-C6-O6
3	p	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	g	401	NAG	C1-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	i	403	NAG	1	0
3	c	403	NAG	1	0
3	m	401	NAG	1	0
3	h	401	NAG	1	0
3	p	401	NAG	1	0
3	k	401	NAG	1	0
3	r	403	NAG	1	0
3	a	401	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

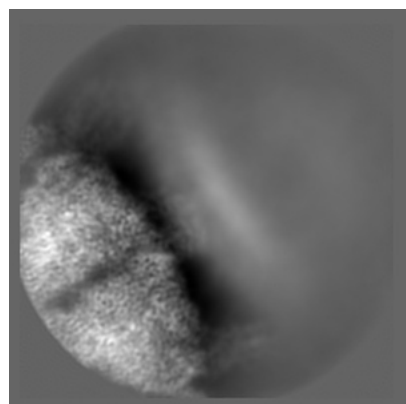
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42343. These allow visual inspection of the internal detail of the map and identification of artifacts.

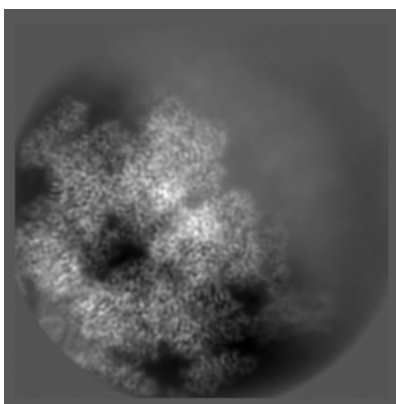
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

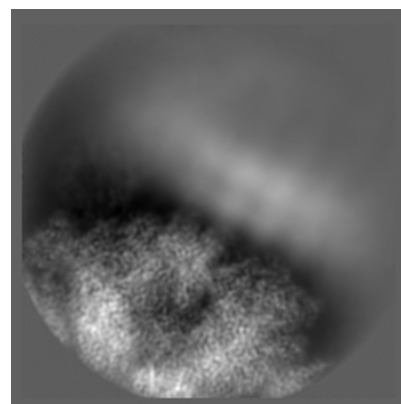
6.1.1 Primary map



X

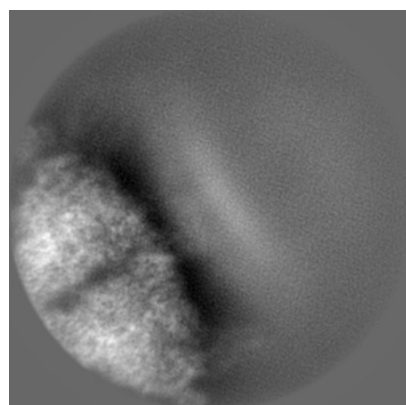


Y

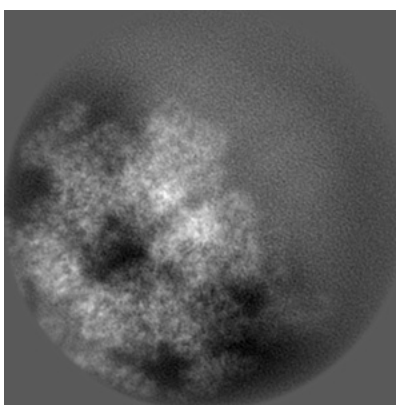


Z

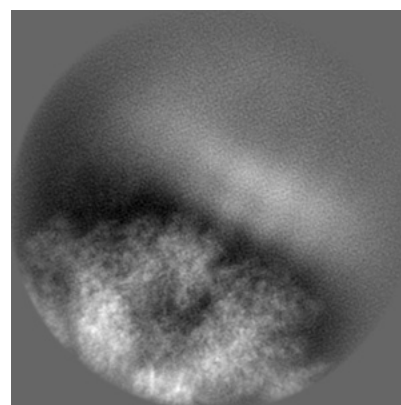
6.1.2 Raw map



X



Y

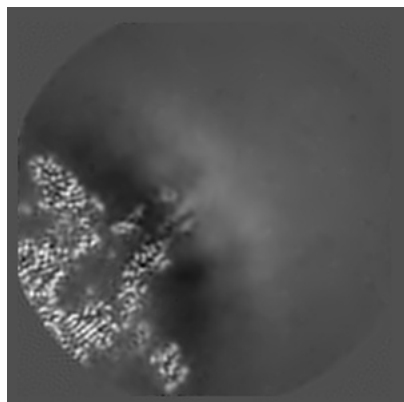


Z

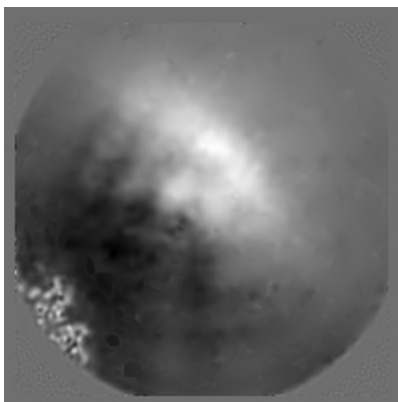
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

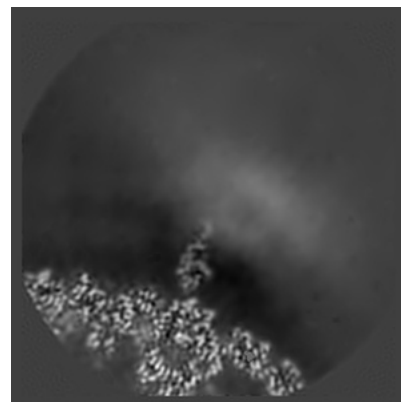
6.2.1 Primary map



X Index: 128

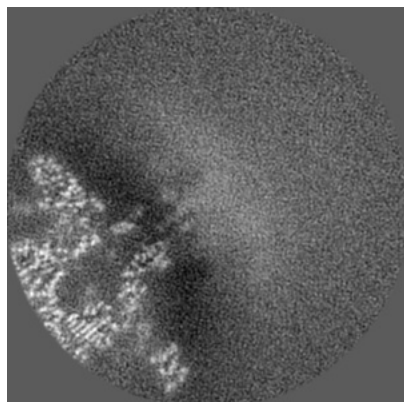


Y Index: 128

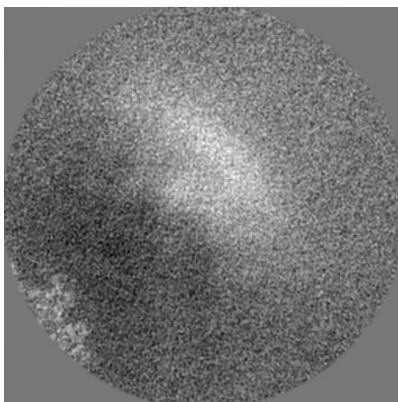


Z Index: 128

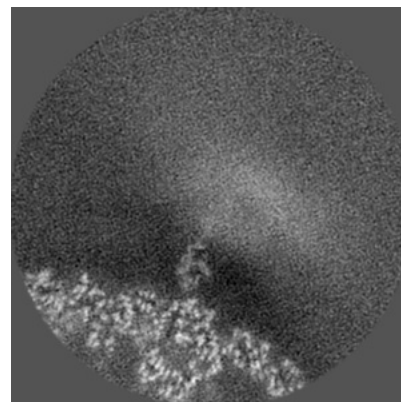
6.2.2 Raw map



X Index: 128



Y Index: 128

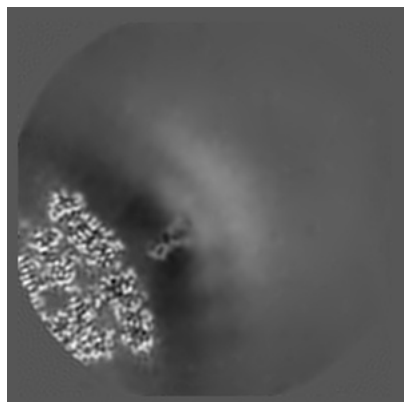


Z Index: 128

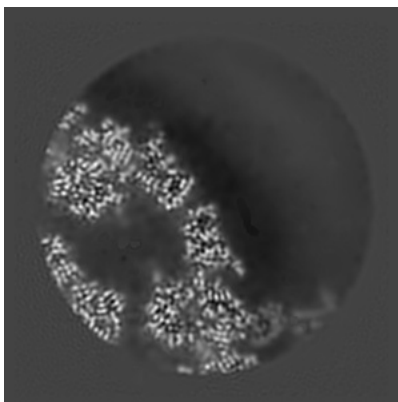
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

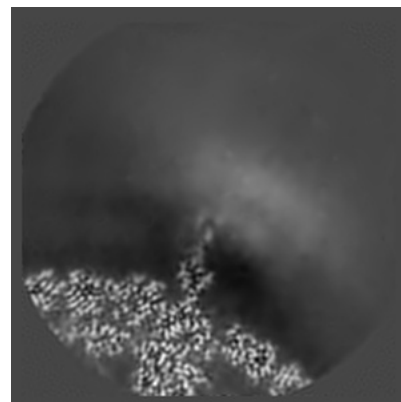
6.3.1 Primary map



X Index: 143

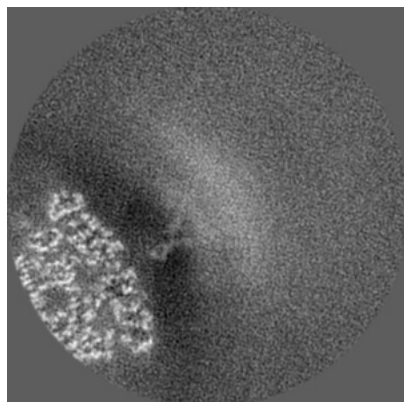


Y Index: 55

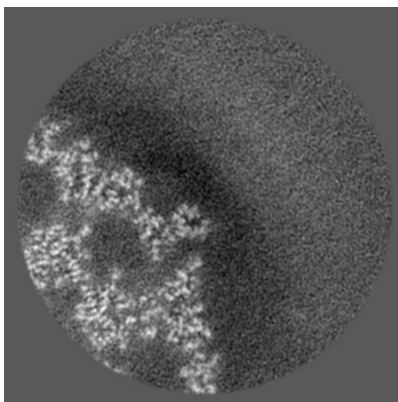


Z Index: 123

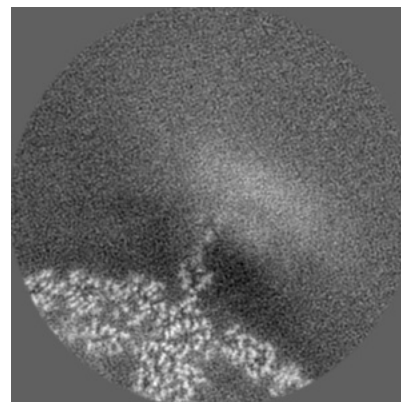
6.3.2 Raw map



X Index: 143



Y Index: 79

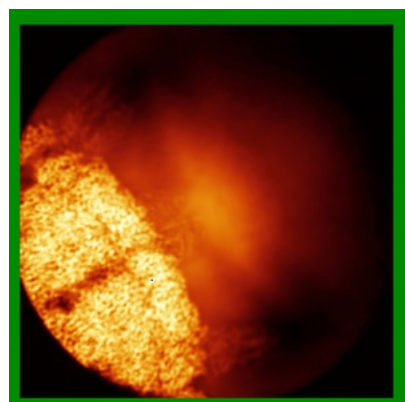


Z Index: 123

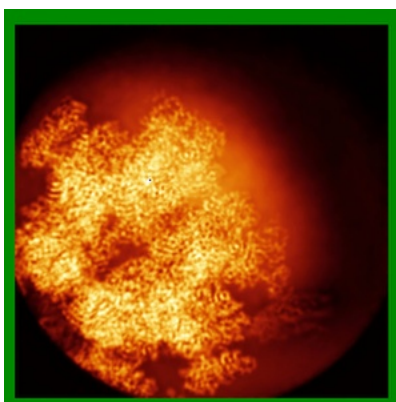
The images above show the largest variance slices of the map in three orthogonal directions.

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

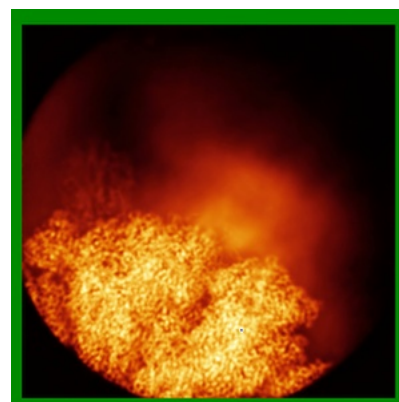
6.4.1 Primary map



X

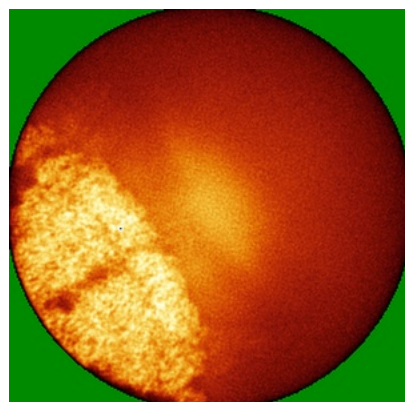


Y

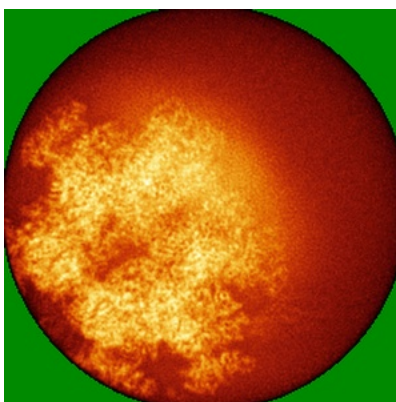


Z

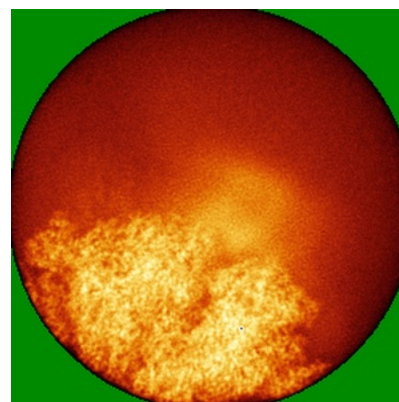
6.4.2 Raw map



X



Y

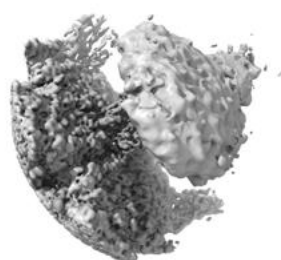


Z

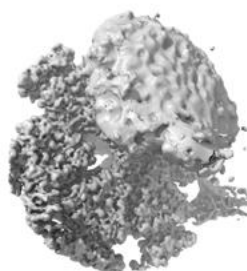
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

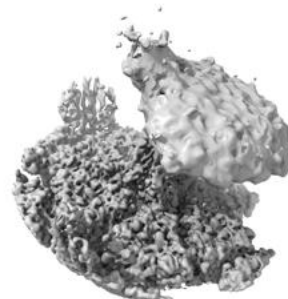
6.5.1 Primary map



X



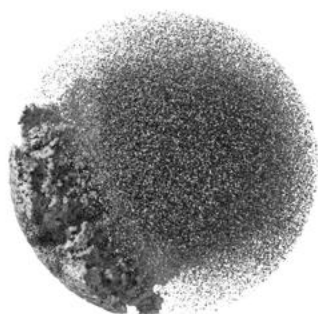
Y



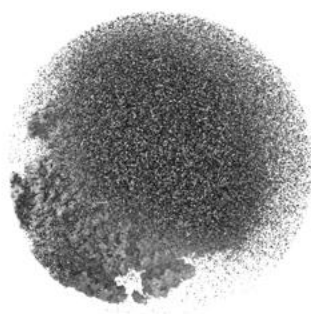
Z

The images above show the 3D surface view of the map at the recommended contour level 0.002. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

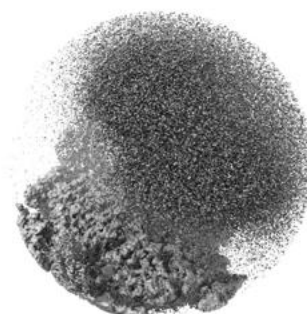
6.5.2 Raw map



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.

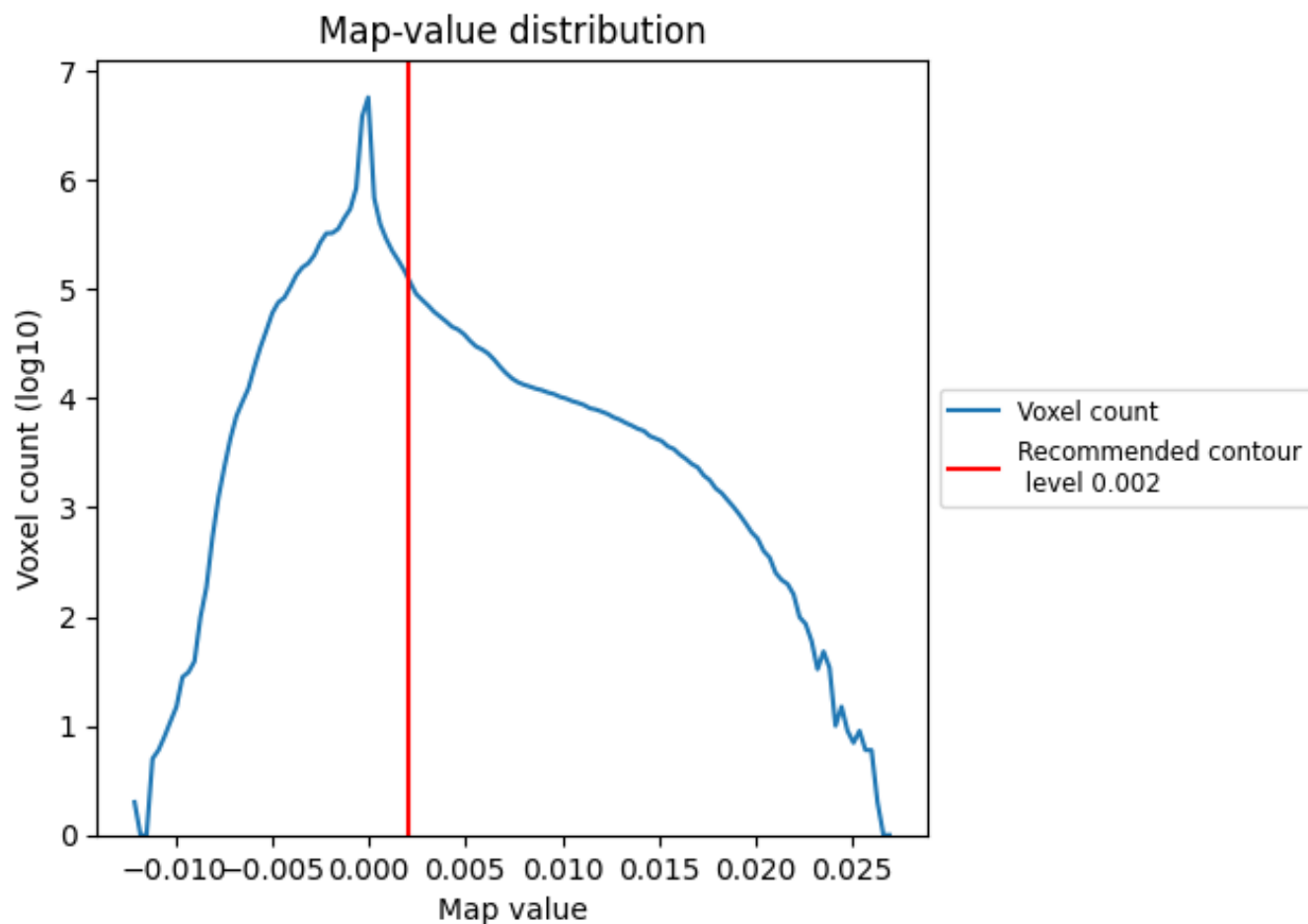
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

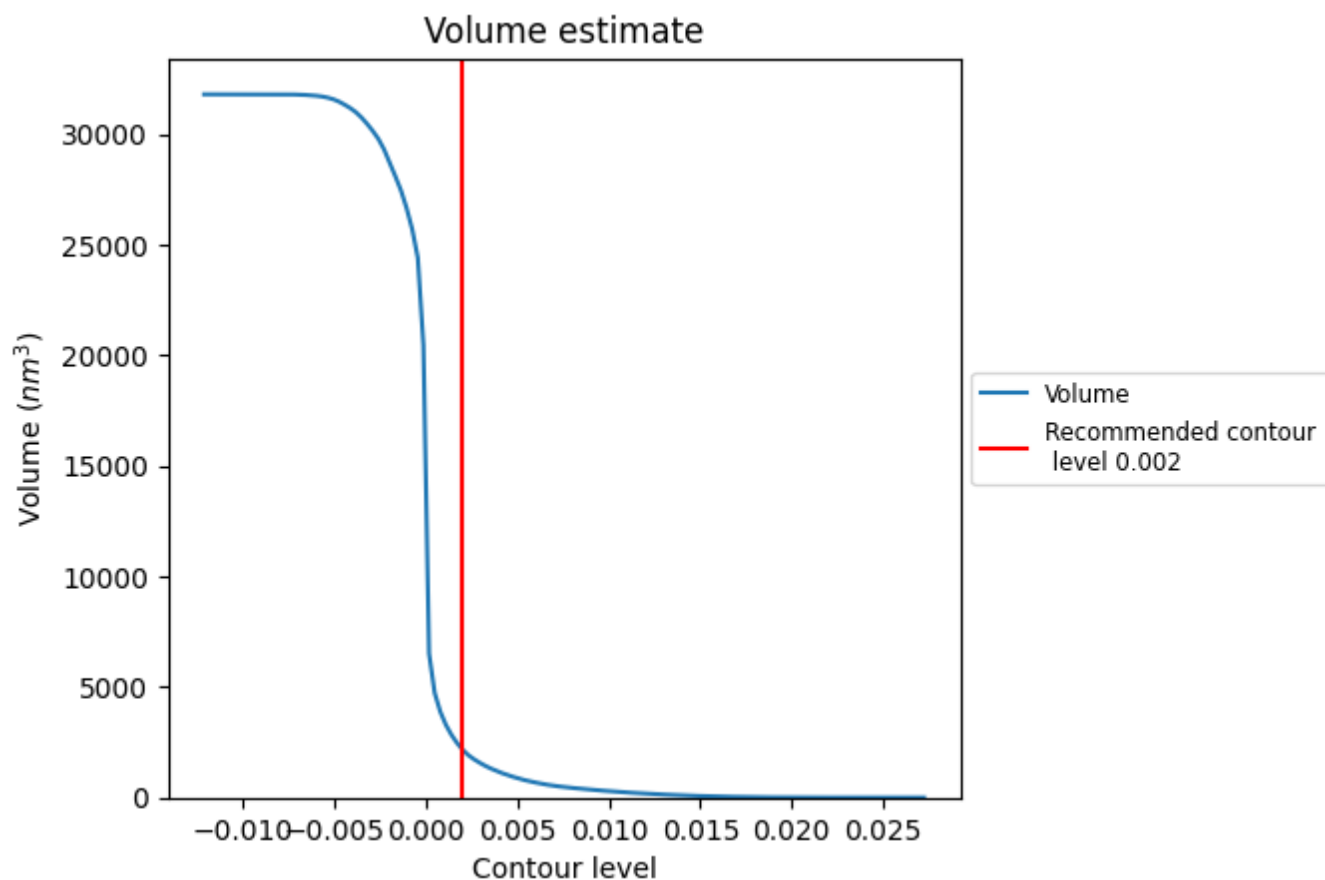
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

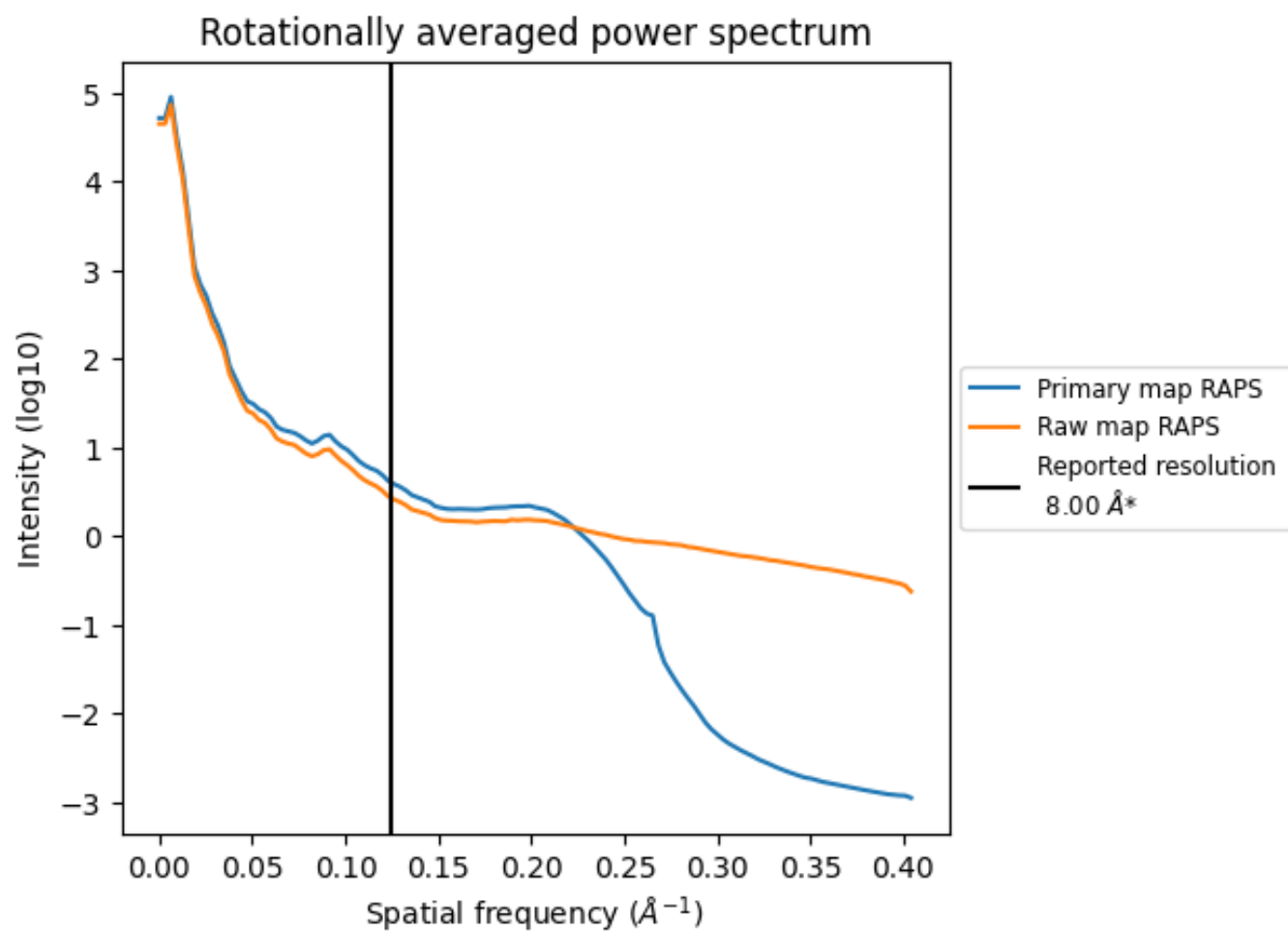
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2187 nm^3 ; this corresponds to an approximate mass of 1976 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

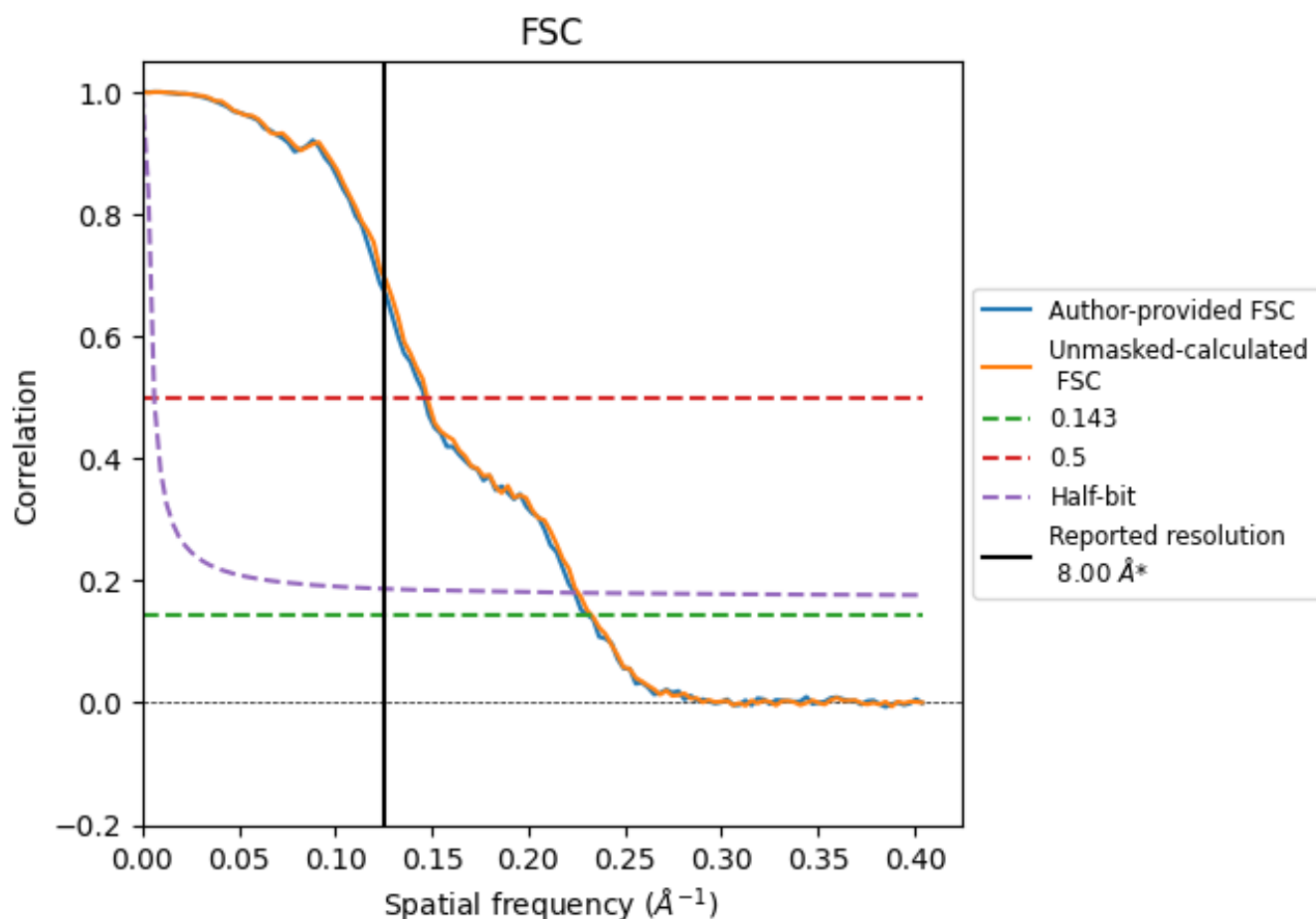


*Reported resolution corresponds to spatial frequency of 0.125 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.125 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

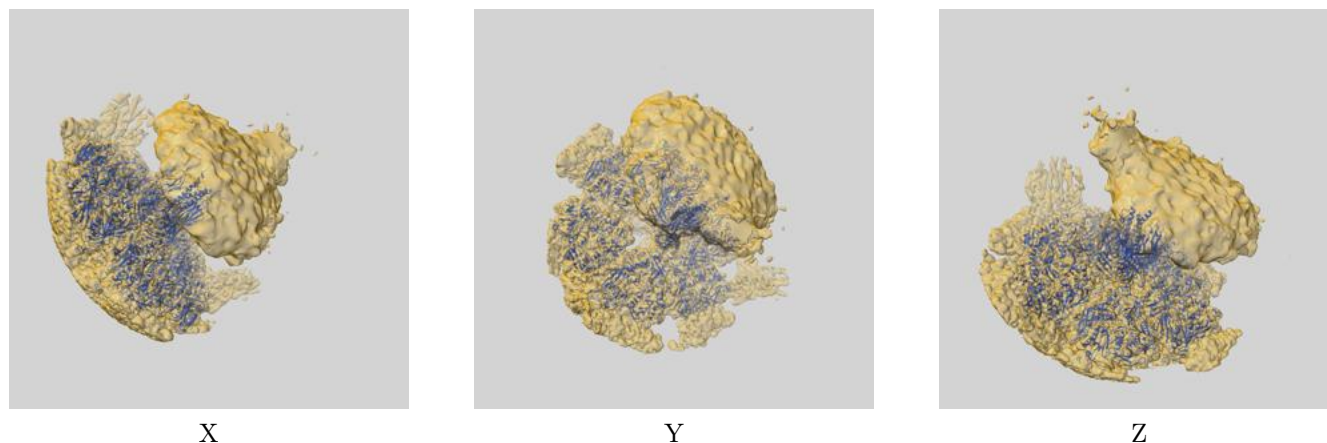
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	8.00
Author-provided FSC curve	4.33	6.84	4.46	-
Unmasked-calculated*	4.30	6.78	4.43	-

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

9 Map-model fit [i](#)

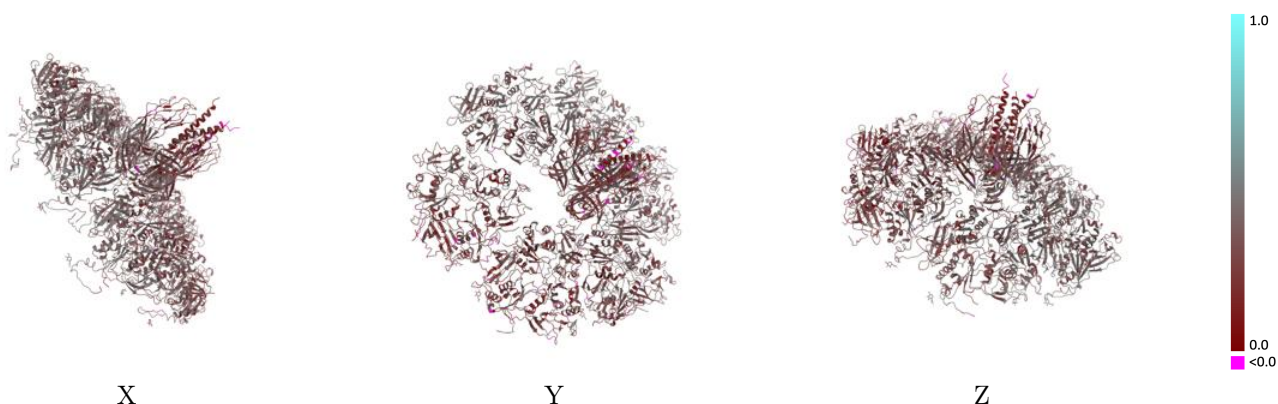
This section contains information regarding the fit between EMDB map EMD-42343 and PDB model 8UK2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



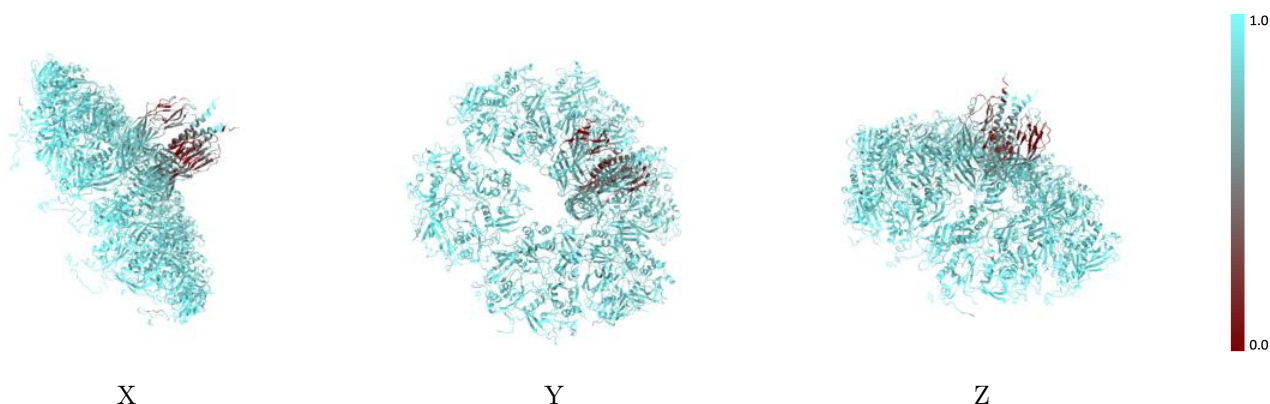
The images above show the 3D surface view of the map at the recommended contour level 0.002 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



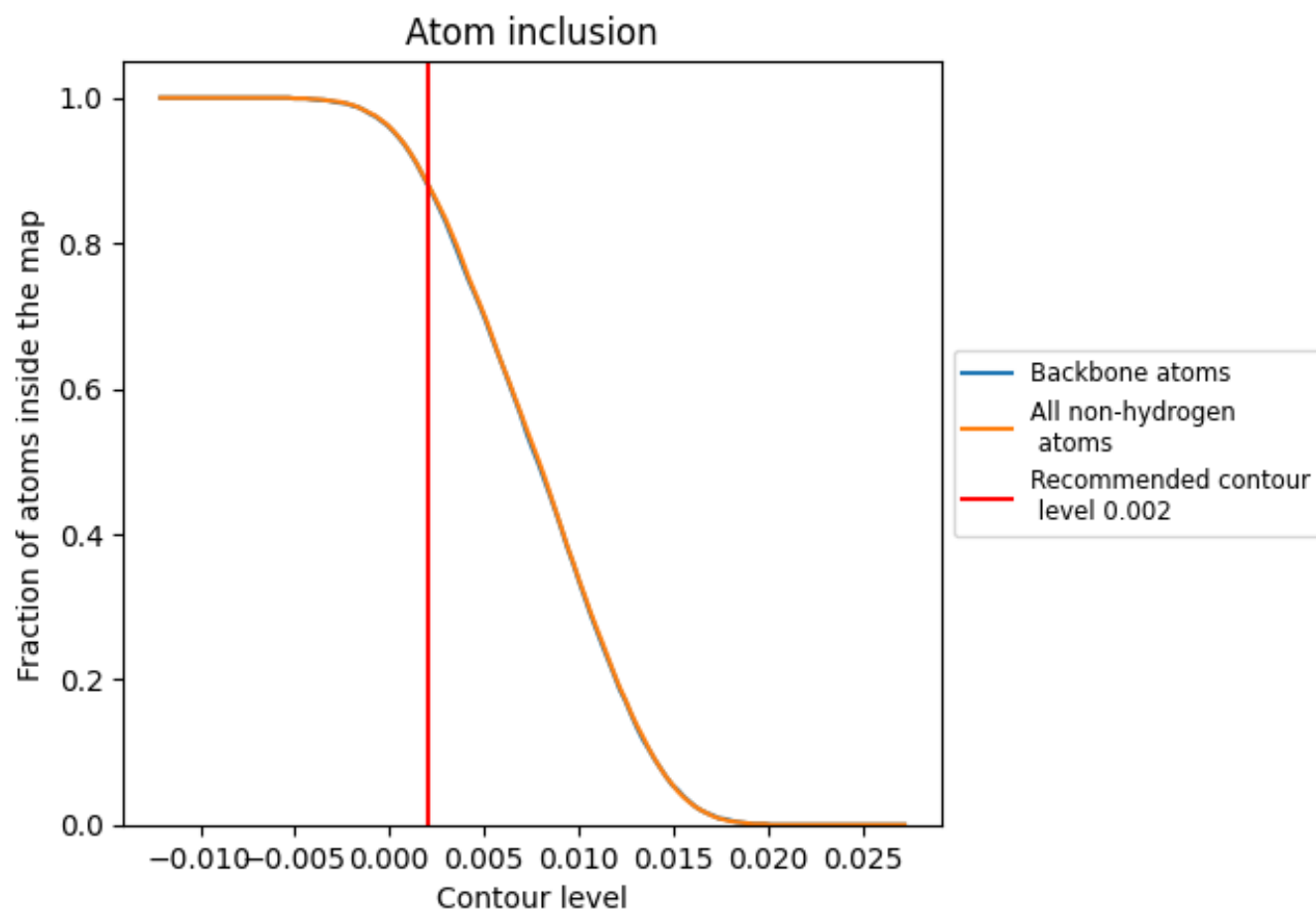
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.002).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.3260
1	 0.6840	 0.2680
2	 0.6630	 0.2900
3	 0.5920	 0.2890
a	 0.9250	 0.3530
b	 0.9420	 0.3740
c	 0.9540	 0.3740
d	 0.9430	 0.3840
e	 0.9620	 0.3910
f	 0.9440	 0.3890
g	 0.9250	 0.3430
h	 0.9350	 0.3500
i	 0.9340	 0.3740
j	 0.9160	 0.2930
k	 0.9230	 0.3350
l	 0.9180	 0.3130
m	 0.9140	 0.2930
n	 0.8970	 0.2880
o	 0.9120	 0.2620
p	 0.9140	 0.2940
q	 0.9200	 0.3250
r	 0.9110	 0.2790

