Full wwPDB EM Validation Report

Oct 14, 2024 – 11:46 AM EDT

PDB ID	:	8UK3
EMDB ID	:	EMD-42344
Title	:	The rotavirus VP5*/VP8* conformational transition permeabilizes membranes to Ca2+ (class 6 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

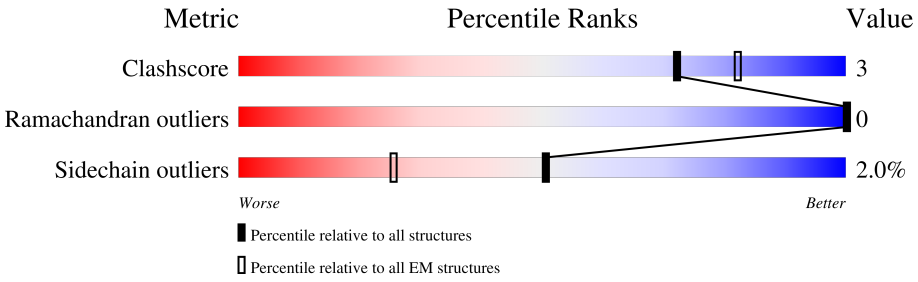
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1	776	31% 5% 65%
1	2	776	32% · 65%
1	3	776	31% · 65%
2	a	326	79% · 21%
2	b	326	83% · 17%
2	c	326	79% · 20%
2	d	326	80% · 19%
2	e	326	79% · 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	f	326	80% 19%
2	g	326	82% 17%
2	h	326	79% 21%
2	i	326	82% 17%
2	j	326	81% 17%
2	k	326	80% 19%
2	l	326	79% 19%
2	m	326	82% 17%
2	n	326	80% 19%
2	o	326	79% 19%
2	p	326	81% 17%
2	q	326	78% 21%
2	r	326	82% 17%

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.

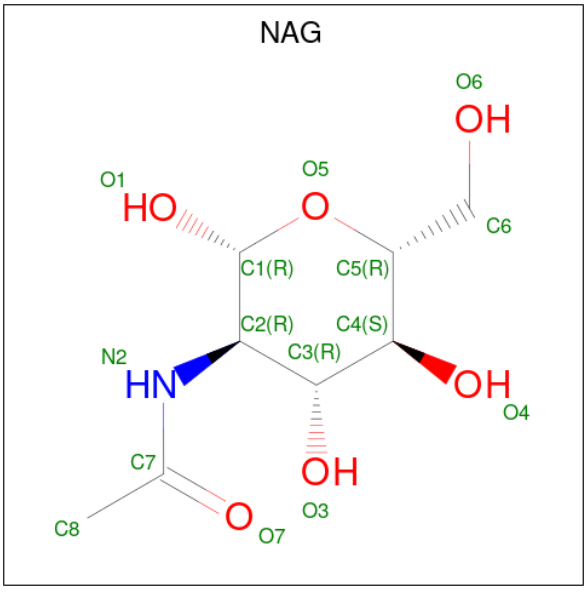
Mol	Chain	Residues	Atoms						AltConf	Trace
2	f	265	Total	C	H	N	O	S	0	0
			4133	1328	2037	333	419	16		
2	g	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	h	259	Total	C	H	N	O	S	0	0
			4041	1298	1994	324	409	16		
2	i	272	Total	C	H	N	O	S	0	0
			4254	1369	2099	342	428	16		
2	j	272	Total	C	H	N	O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

Continued on next page...

Continued from previous page...

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 (three-letter code: 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	

Continued on next page...

Continued from previous page...

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 (three-letter code: 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	

Continued on next page...

Continued from previous page...

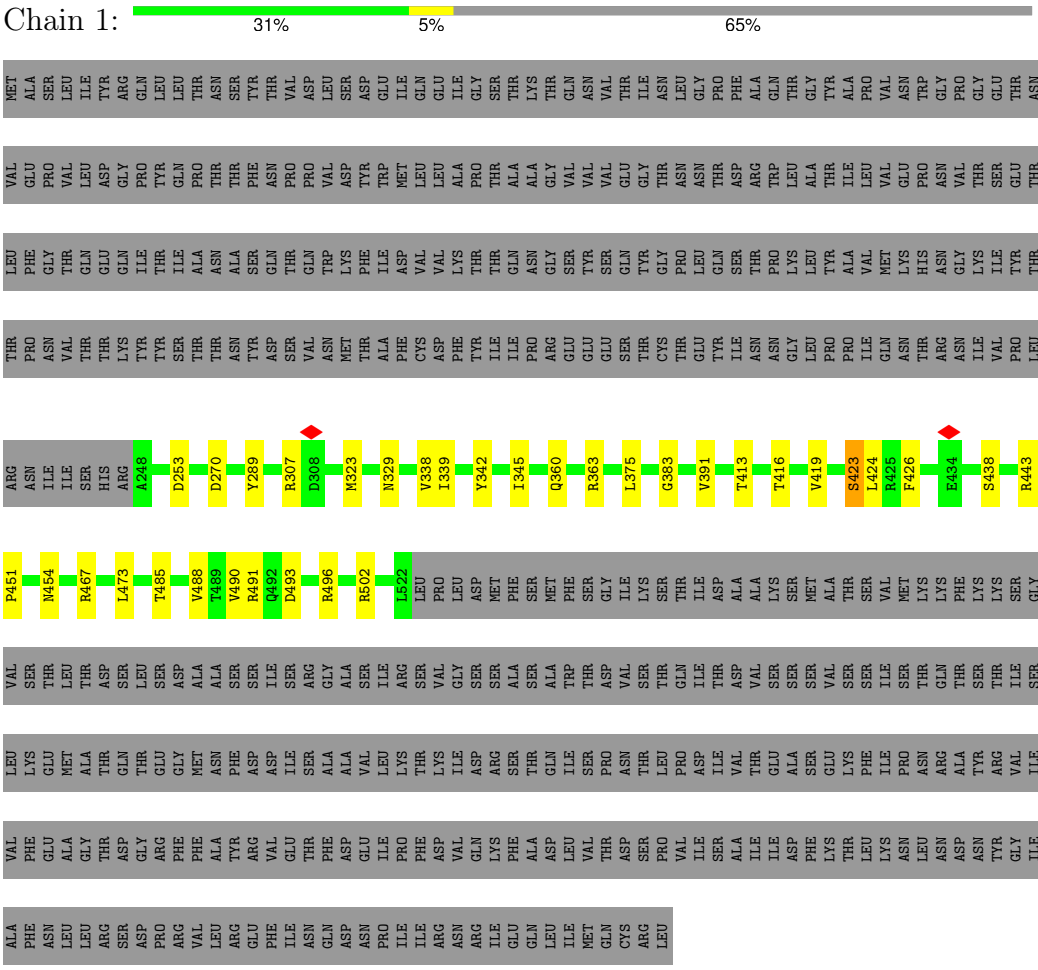
Mol	Chain	Residues	Atoms	AltConf
4	l	3	Total Ca 3 3	0
4	m	3	Total Ca 3 3	0
4	n	3	Total Ca 3 3	0
4	o	3	Total Ca 3 3	0
4	p	3	Total Ca 3 3	0
4	q	3	Total Ca 3 3	0
4	r	3	Total Ca 3 3	0
4	a	3	Total Ca 3 3	0
4	b	3	Total Ca 3 3	0
4	c	3	Total Ca 3 3	0
4	d	3	Total Ca 3 3	0
4	e	3	Total Ca 3 3	0

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.

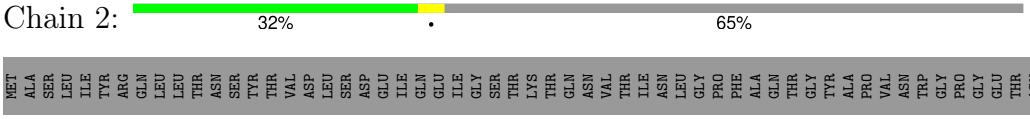
• Molecule 1: Outer capsid protein VP4

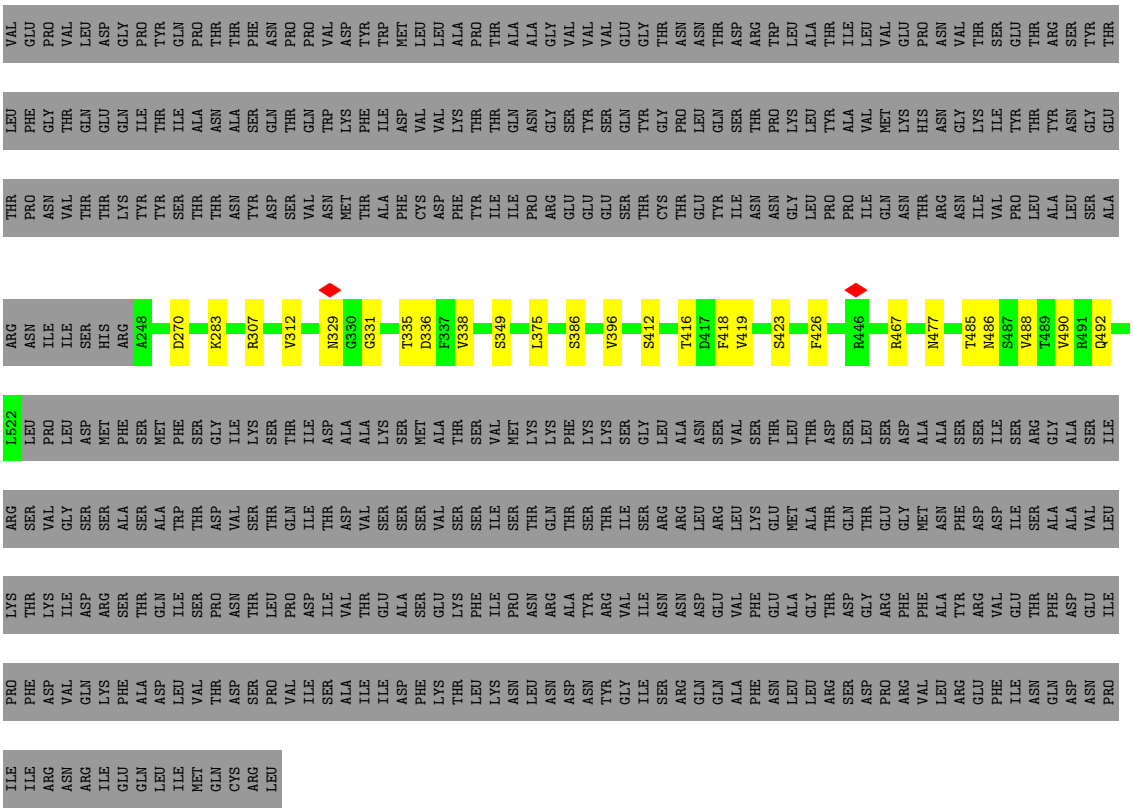
Chain 1:



• Molecule 1: Outer capsid protein VP4

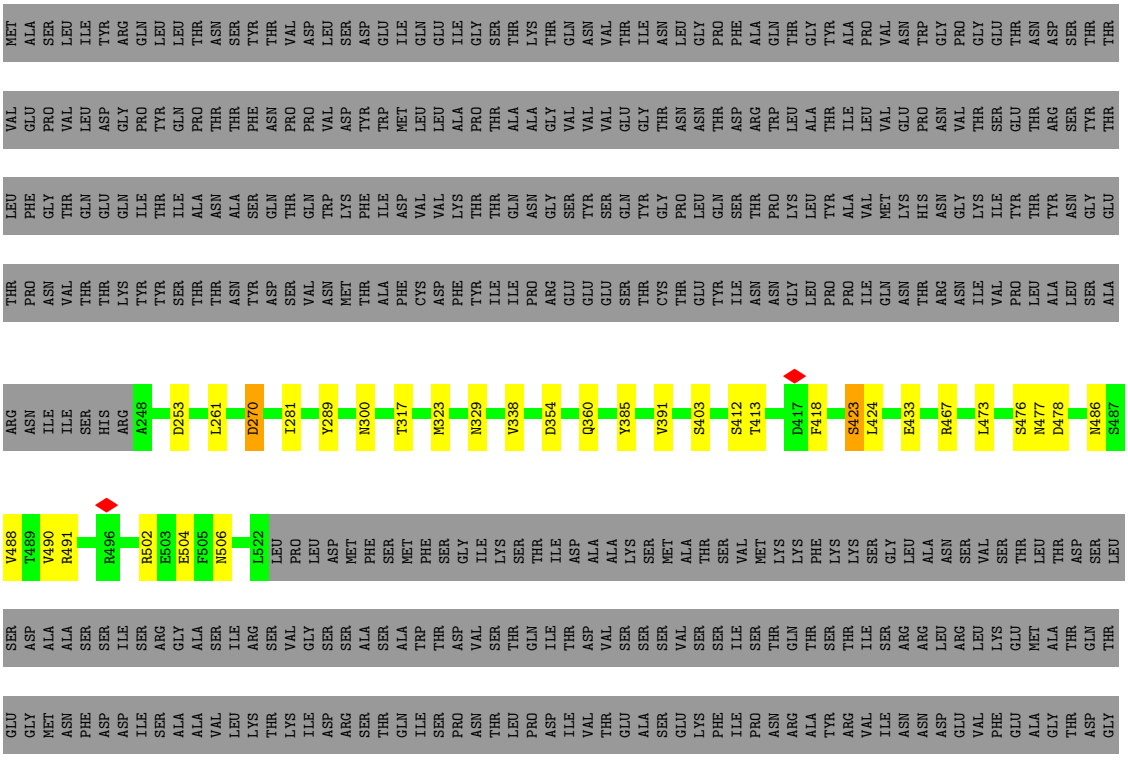
Chain 2:

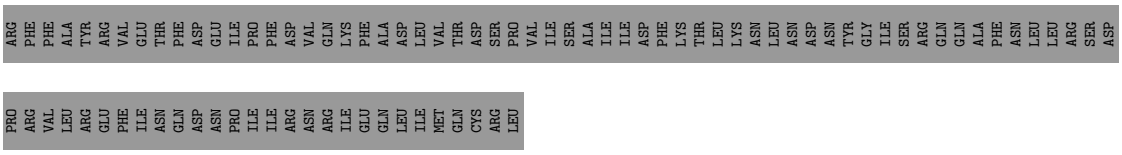




• Molecule 1: Outer capsid protein VP4

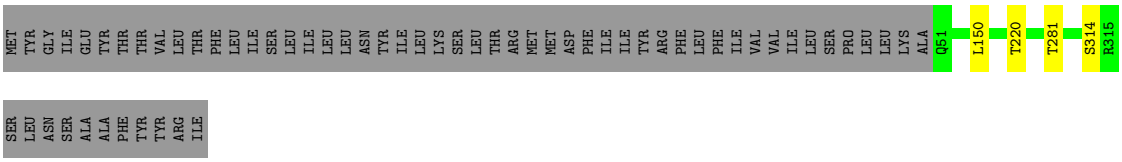
Chain 3:





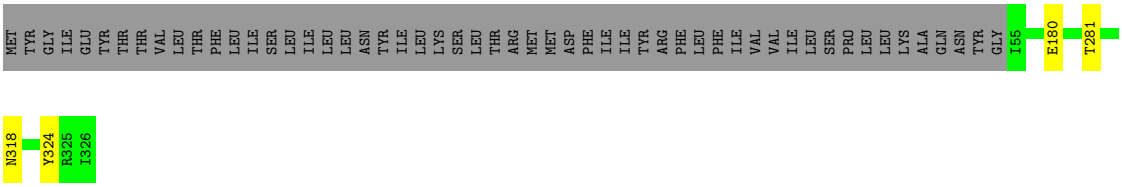
• Molecule 2: Outer capsid glycoprotein VP7

Chain f:



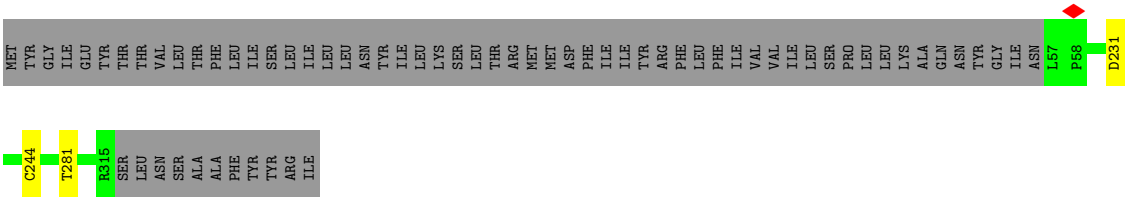
• Molecule 2: Outer capsid glycoprotein VP7

Chain g:



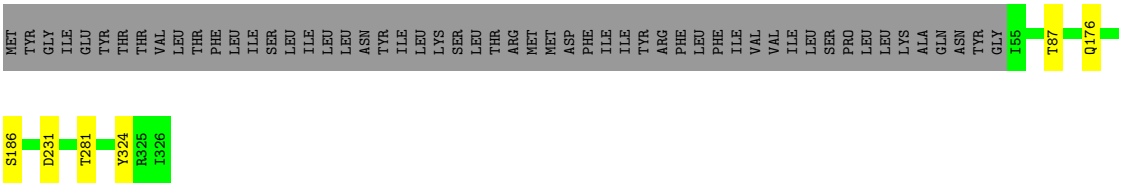
• Molecule 2: Outer capsid glycoprotein VP7

Chain h:



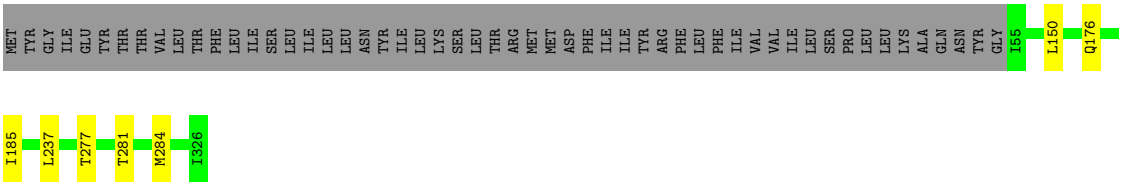
• Molecule 2: Outer capsid glycoprotein VP7

Chain i:



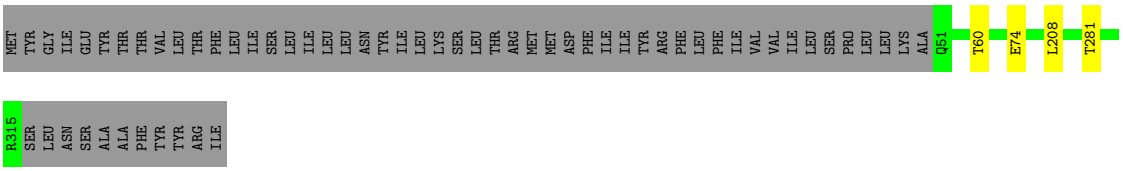
• Molecule 2: Outer capsid glycoprotein VP7

Chain j:



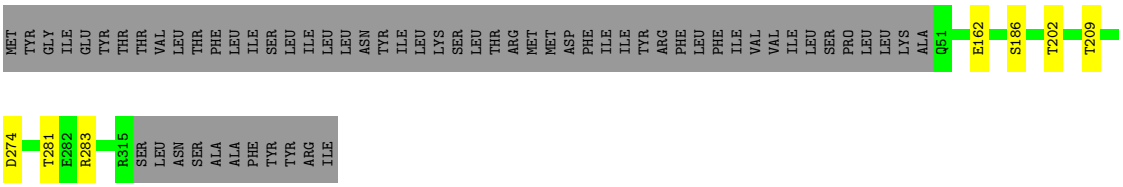
• Molecule 2: Outer capsid glycoprotein VP7

Chain k:



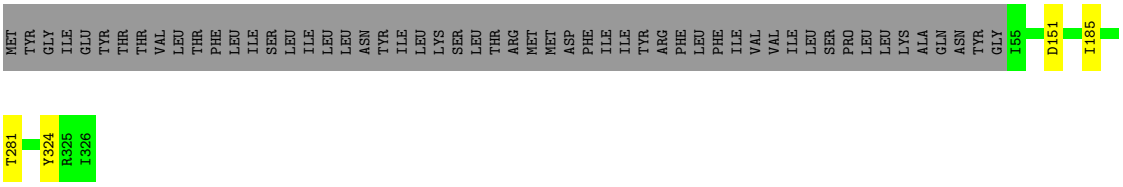
• Molecule 2: Outer capsid glycoprotein VP7

Chain l:



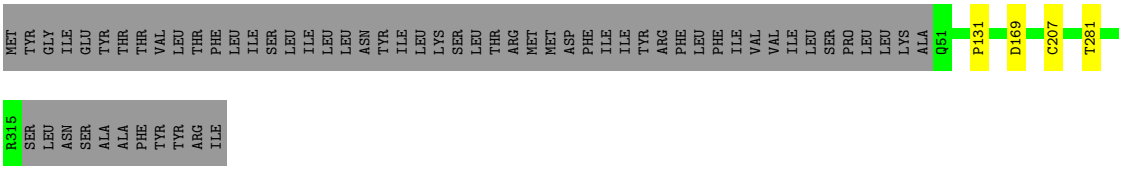
• Molecule 2: Outer capsid glycoprotein VP7

Chain m:



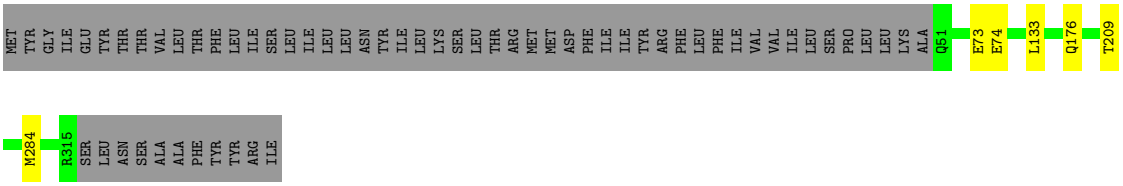
• Molecule 2: Outer capsid glycoprotein VP7

Chain n:

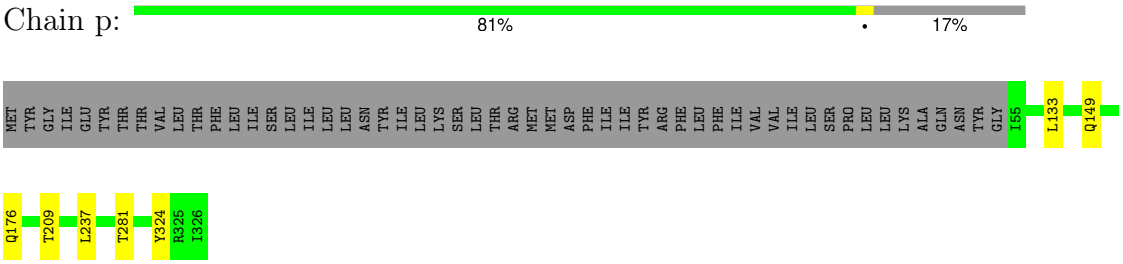


• Molecule 2: Outer capsid glycoprotein VP7

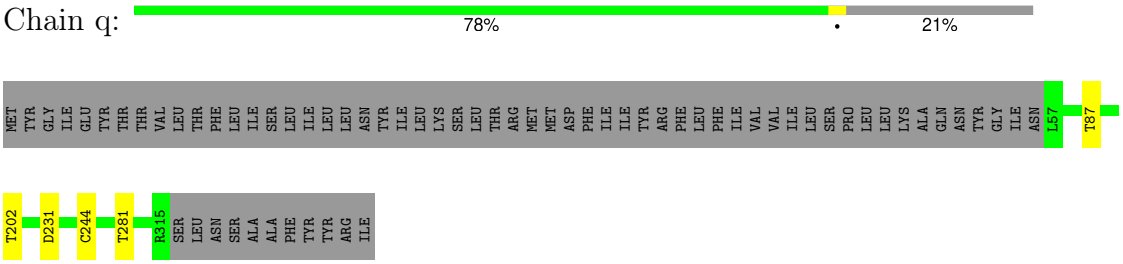
Chain o:



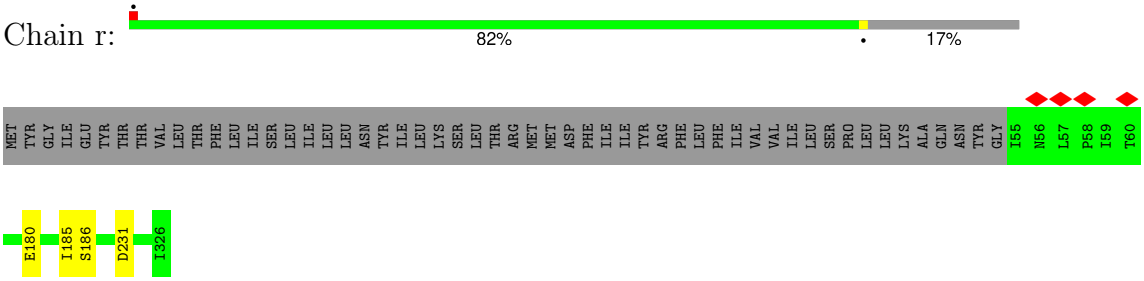
• Molecule 2: Outer capsid glycoprotein VP7



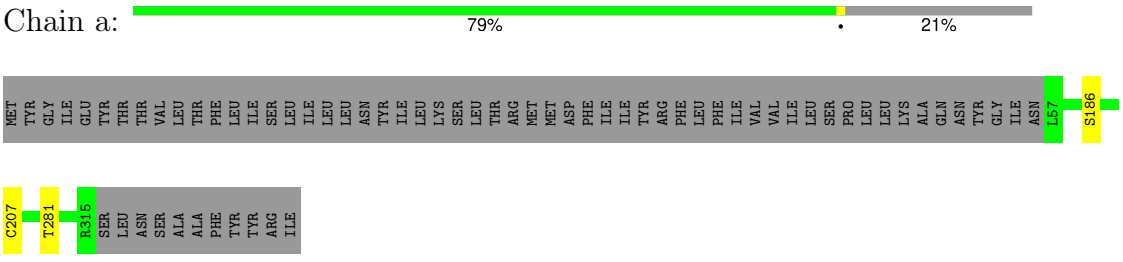
• Molecule 2: Outer capsid glycoprotein VP7



• Molecule 2: Outer capsid glycoprotein VP7

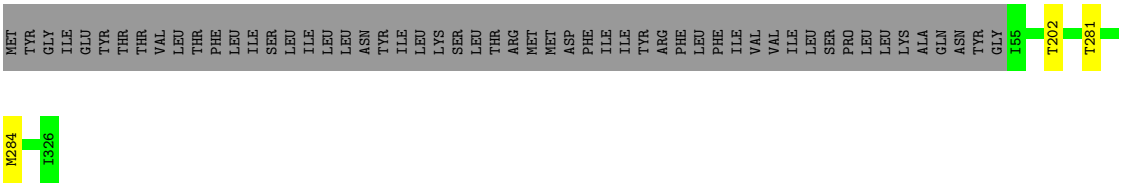


• Molecule 2: Outer capsid glycoprotein VP7



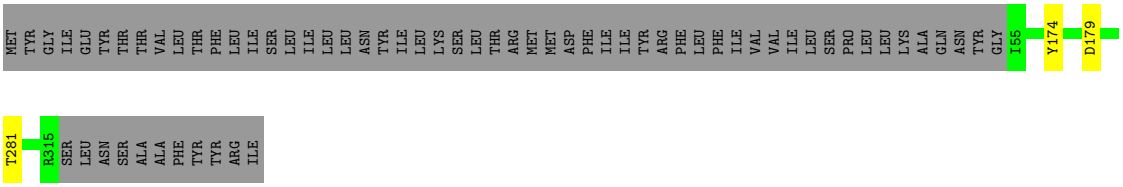
• Molecule 2: Outer capsid glycoprotein VP7

Chain b:



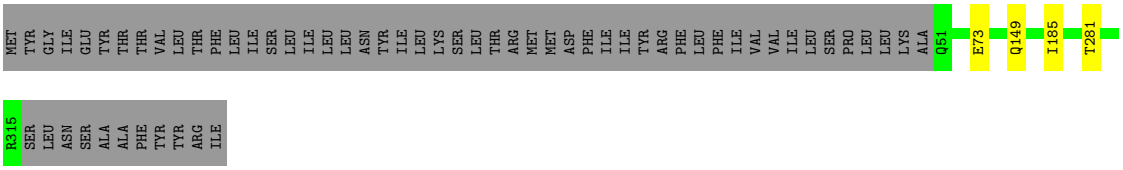
• Molecule 2: Outer capsid glycoprotein VP7

Chain c:



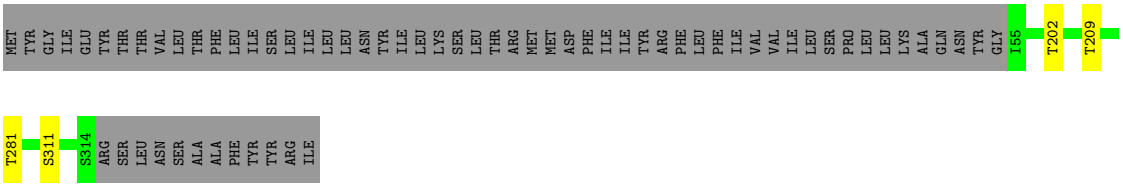
• Molecule 2: Outer capsid glycoprotein VP7

Chain d:



• Molecule 2: Outer capsid glycoprotein VP7

Chain e:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70018	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 ($e^-/Å^2$)	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	0.030	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	0.27	0/2232	0.57	0/3032
1	2	0.27	0/2232	0.57	0/3032
1	3	0.27	0/2232	0.57	0/3032
2	a	0.27	0/2089	0.55	0/2854
2	b	0.26	0/2200	0.54	0/3005
2	c	0.27	0/2105	0.54	0/2876
2	d	0.27	0/2139	0.54	0/2922
2	e	0.27	0/2094	0.54	0/2862
2	f	0.27	0/2139	0.53	0/2922
2	g	0.27	0/2200	0.55	0/3005
2	h	0.27	0/2089	0.54	0/2854
2	i	0.28	0/2200	0.55	0/3005
2	j	0.27	0/2200	0.54	0/3005
2	k	0.27	0/2139	0.56	0/2922
2	l	0.27	0/2139	0.55	0/2922
2	m	0.27	0/2200	0.55	0/3005
2	n	0.26	0/2139	0.55	0/2922
2	o	0.27	0/2139	0.54	0/2922
2	p	0.27	0/2200	0.55	0/3005
2	q	0.27	0/2089	0.54	0/2854
2	r	0.27	0/2200	0.55	0/3005
All	All	0.27	0/45396	0.55	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	20	0
2	a	2047	1994	1993	0	0
2	b	2155	2099	2099	0	0
2	c	2063	2011	2010	0	0
2	d	2096	2037	2036	0	0
2	e	2052	1998	1997	0	0
2	f	2096	2037	2036	0	0
2	g	2155	2099	2098	0	0
2	h	2047	1994	1993	0	0
2	i	2155	2099	2098	0	0
2	j	2155	2099	2098	0	0
2	k	2096	2037	2036	0	0
2	l	2096	2037	2036	0	0
2	m	2155	2099	2098	0	0
2	n	2096	2037	2036	0	0
2	o	2096	2037	2036	0	0
2	p	2155	2099	2098	0	0
2	q	2047	1994	1993	0	0
2	r	2155	2099	2098	0	0
3	a	14	14	13	0	0
3	b	14	14	13	0	0
3	c	14	14	13	0	0
3	d	14	14	13	0	0
3	e	14	14	13	0	0
3	f	14	14	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	g	14	14	13	0	0
3	h	14	14	13	0	0
3	i	14	14	13	0	0
3	j	14	14	13	0	0
3	k	14	14	13	0	0
3	l	14	14	13	0	0
3	m	14	14	13	0	0
3	n	14	14	13	0	0
3	o	14	14	13	0	0
3	p	14	14	13	0	0
3	q	14	14	13	0	0
3	r	14	14	13	0	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	47	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 3.

All (47) 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
1:3:270:ASP:OD1	1:3:467:ARG:NH1	2.23	0.72
1:2:485:THR:HG1	1:3:412:SER:HG	1.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:493:ASP:OD1	1:1:496:ARG:NH2	2.27	0.68
1:1:485:THR:OG1	1:2:412:SER:OG	2.08	0.67
1:1:491:ARG:NH2	1:2:492:GLN:OE1	2.30	0.65
1:1:360:GLN:OE1	1:1:363:ARG:NH1	2.30	0.64
1:1:502:ARG:NH2	1:2:283:LYS:O	2.35	0.60
1:2:485:THR:OG1	1:3:412:SER:OG	2.17	0.59
1:1:270:ASP:OD1	1:1:467:ARG:NH1	2.35	0.59
1:3:300:ASN:ND2	1:3:317:THR:OG1	2.37	0.57
1:3:403:SER:OG	1:3:433:GLU:OE2	2.23	0.56
1:2:416:THR:OG1	1:2:419:VAL:O	2.22	0.55
1:1:502:ARG:NH1	1:3:504:GLU:OE1	2.40	0.53
1:3:360:GLN:NE2	1:3:478:ASP:OD1	2.42	0.52
1:3:281:ILE:HG21	1:3:385:TYR:OH	2.10	0.52
1:1:490:VAL:O	1:3:491:ARG:NE	2.40	0.51
1:3:253:ASP:OD1	1:3:253:ASP:N	2.44	0.50
1:1:450:LEU:HD12	1:1:451:PRO:HD2	1.94	0.50
1:1:383:GLY:N	1:1:454:ASN:O	2.44	0.50
1:1:253:ASP:OD1	1:1:253:ASP:N	2.45	0.49
1:3:418:PHE:O	1:3:486:ASN:N	2.44	0.49
1:3:270:ASP:OD1	1:3:270:ASP:N	2.45	0.48
1:2:329:ASN:HA	1:2:338:VAL:HG23	1.95	0.48
1:1:345:ILE:HD12	1:1:450:LEU:HD23	1.95	0.47
1:3:329:ASN:HA	1:3:338:VAL:HG23	1.96	0.47
1:2:331:GLY:N	1:2:336:ASP:OD2	2.47	0.47
1:1:438:SER:OG	1:1:444:VAL:O	2.32	0.47
1:2:270:ASP:OD1	1:2:467:ARG:NH1	2.47	0.47
1:1:329:ASN:HA	1:1:338:VAL:HG23	1.98	0.46
1:1:416:THR:OG1	1:1:419:VAL:O	2.27	0.45
1:2:386:SER:HA	1:2:396:VAL:HG12	1.99	0.45
1:1:339:ILE:HD12	1:1:342:TYR:CD2	2.52	0.44
1:3:289:TYR:OH	1:3:391:VAL:O	2.26	0.44
1:1:289:TYR:OH	1:1:391:VAL:O	2.24	0.44
1:3:488:VAL:HG12	1:3:490:VAL:H	1.82	0.43
1:2:418:PHE:O	1:2:486:ASN:N	2.50	0.43
1:2:375:LEU:HD11	1:2:426:PHE:CD1	2.54	0.42
1:2:488:VAL:HG13	1:2:490:VAL:HG23	2.01	0.42
1:1:375:LEU:HD11	1:1:426:PHE:CD1	2.55	0.41
1:1:270:ASP:OD1	1:1:270:ASP:N	2.54	0.41
1:1:488:VAL:HG11	1:3:490:VAL:CG2	2.51	0.41
1:3:423:SER:OG	1:3:424:LEU:N	2.54	0.41
1:3:354:ASP:N	1:3:354:ASP:OD1	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:502:ARG:O	1:3:506:ASN:ND2	2.53	0.40
1:1:423:SER:OG	1:1:424:LEU:N	2.52	0.40
1:3:261:LEU:O	1:3:476:SER:N	2.47	0.40

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	o	263/326 (81%)	263 (100%)	0	0	100	100
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	241/688 (35%)	235 (98%)	6 (2%)	42	61
1	2	241/688 (35%)	235 (98%)	6 (2%)	42	61
1	3	241/688 (35%)	235 (98%)	6 (2%)	42	61
2	a	233/295 (79%)	230 (99%)	3 (1%)	65	77
2	b	244/295 (83%)	241 (99%)	3 (1%)	67	78
2	c	235/295 (80%)	232 (99%)	3 (1%)	65	77
2	d	238/295 (81%)	234 (98%)	4 (2%)	56	72
2	e	234/295 (79%)	231 (99%)	3 (1%)	65	77
2	f	238/295 (81%)	234 (98%)	4 (2%)	56	72
2	g	244/295 (83%)	240 (98%)	4 (2%)	58	73
2	h	233/295 (79%)	230 (99%)	3 (1%)	65	77
2	i	244/295 (83%)	238 (98%)	6 (2%)	42	61
2	j	244/295 (83%)	237 (97%)	7 (3%)	37	56
2	k	238/295 (81%)	234 (98%)	4 (2%)	56	72
2	l	238/295 (81%)	231 (97%)	7 (3%)	37	56
2	m	244/295 (83%)	240 (98%)	4 (2%)	58	73
2	n	238/295 (81%)	234 (98%)	4 (2%)	56	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	o	238/295 (81%)	232 (98%)	6 (2%)	42	61
2	p	244/295 (83%)	237 (97%)	7 (3%)	37	56
2	q	233/295 (79%)	228 (98%)	5 (2%)	48	66
2	r	244/295 (83%)	240 (98%)	4 (2%)	58	73
All	All	5027/7374 (68%)	4928 (98%)	99 (2%)	50	68

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	307	ARG
1	1	323	MET
1	1	413	THR
1	1	423	SER
1	1	443	ARG
1	1	473	LEU
2	f	150	LEU
2	f	220	THR
2	f	281	THR
2	f	314	SER
1	2	307	ARG
1	2	312	VAL
1	2	335	THR
1	2	349	SER
1	2	423	SER
1	2	477	ASN
2	g	180	GLU
2	g	281	THR
2	g	318	ASN
2	g	324	TYR
1	3	270	ASP
1	3	323	MET
1	3	413	THR
1	3	423	SER
1	3	473	LEU
1	3	477	ASN
2	h	231	ASP
2	h	244	CYS
2	h	281	THR
2	i	87	THR
2	i	176	GLN
2	i	186	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	i	231	ASP
2	i	281	THR
2	i	324	TYR
2	j	150	LEU
2	j	176	GLN
2	j	185	ILE
2	j	237	LEU
2	j	277	THR
2	j	281	THR
2	j	284	MET
2	k	60	THR
2	k	74	GLU
2	k	208	LEU
2	k	281	THR
2	l	162	GLU
2	l	186	SER
2	l	202	THR
2	l	209	THR
2	l	274	ASP
2	l	281	THR
2	l	283	ARG
2	m	151	ASP
2	m	185	ILE
2	m	281	THR
2	m	324	TYR
2	n	131	PRO
2	n	169	ASP
2	n	207	CYS
2	n	281	THR
2	o	73	GLU
2	o	74	GLU
2	o	133	LEU
2	o	176	GLN
2	o	209	THR
2	o	284	MET
2	p	133	LEU
2	p	149	GLN
2	p	176	GLN
2	p	209	THR
2	p	237	LEU
2	p	281	THR
2	p	324	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	q	87	THR
2	q	202	THR
2	q	231	ASP
2	q	244	CYS
2	q	281	THR
2	r	180	GLU
2	r	185	ILE
2	r	186	SER
2	r	231	ASP
2	a	186	SER
2	a	207	CYS
2	a	281	THR
2	b	202	THR
2	b	281	THR
2	b	284	MET
2	c	174	TYR
2	c	179	ASP
2	c	281	THR
2	d	73	GLU
2	d	149	GLN
2	d	185	ILE
2	d	281	THR
2	e	202	THR
2	e	209	THR
2	e	281	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	f	149	GLN
2	g	132	GLN
2	g	149	GLN
2	g	176	GLN
2	g	234	ASN
2	h	149	GLN
2	h	182	ASN
2	h	248	ASN
2	j	132	GLN
2	j	248	ASN
2	j	305	GLN
2	k	305	GLN
2	l	248	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	n	52	ASN
2	n	288	ASN
2	n	305	GLN
2	r	182	ASN
2	r	248	ASN
2	c	305	GLN
2	d	149	GLN
2	d	176	GLN
2	d	234	ASN

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	o	403	2	14,14,15	0.50	0	17,19,21	0.47	0
3	NAG	q	401	2	14,14,15	0.47	0	17,19,21	0.71	1 (5%)
3	NAG	l	403	2	14,14,15	0.41	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	m	401	2	14,14,15	0.63	1 (7%)	17,19,21	0.73	1 (5%)
3	NAG	p	401	2	14,14,15	0.55	0	17,19,21	0.76	1 (5%)
3	NAG	b	401	-	14,14,15	0.24	0	17,19,21	0.51	0
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	r	403	2	14,14,15	0.65	1 (7%)	17,19,21	0.78	1 (5%)
3	NAG	j	402	2	14,14,15	0.37	0	17,19,21	0.37	0
3	NAG	a	401	2	14,14,15	0.67	1 (7%)	17,19,21	0.78	1 (5%)
3	NAG	i	403	2	14,14,15	0.64	1 (7%)	17,19,21	0.74	1 (5%)
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	g	401	2	14,14,15	0.45	0	17,19,21	0.46	0
3	NAG	n	401	2	14,14,15	0.33	0	17,19,21	0.36	0
3	NAG	k	401	2	14,14,15	0.65	1 (7%)	17,19,21	0.80	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	o	403	2	-	0/6/23/26	0/1/1/1
3	NAG	q	401	2	-	0/6/23/26	0/1/1/1
3	NAG	l	403	2	-	0/6/23/26	0/1/1/1
3	NAG	m	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	b	401	-	-	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
3	NAG	r	403	2	-	0/6/23/26	0/1/1/1
3	NAG	j	402	2	-	0/6/23/26	0/1/1/1
3	NAG	a	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	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	g	401	2	-	1/6/23/26	0/1/1/1
3	NAG	n	401	2	-	0/6/23/26	0/1/1/1
3	NAG	k	401	2	-	0/6/23/26	0/1/1/1

All (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
3	h	401	NAG	C1-C2	2.20	1.55	1.52
3	c	403	NAG	C1-C2	2.13	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
3	h	401	NAG	C1-O5-C5	2.55	115.61	112.19
3	m	401	NAG	C1-O5-C5	2.54	115.59	112.19
3	c	403	NAG	C1-O5-C5	2.45	115.46	112.19
3	q	401	NAG	C1-O5-C5	2.37	115.37	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
3	g	401	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

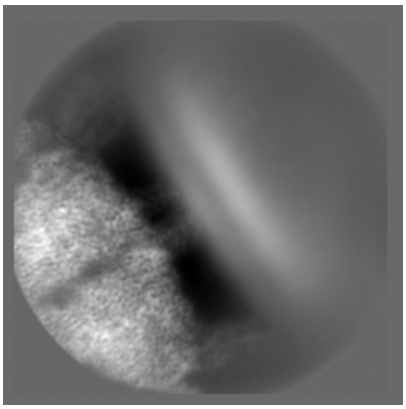
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42344. These allow visual inspection of the internal detail of the map and identification of artifacts.

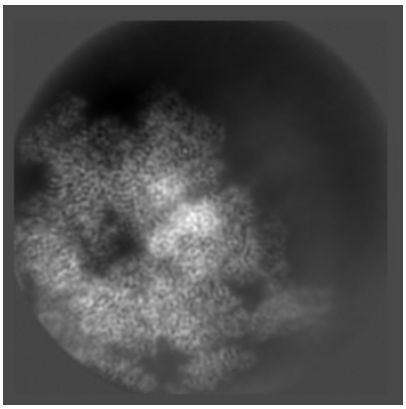
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

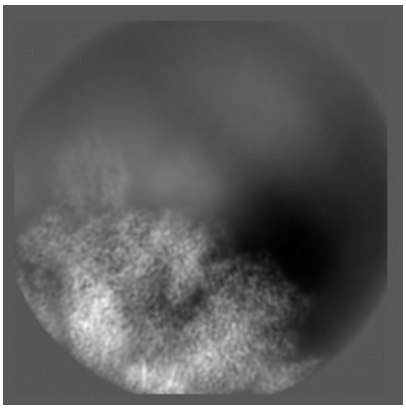
6.1.1 Primary map



X

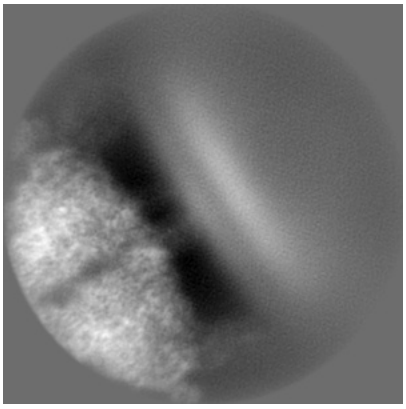


Y

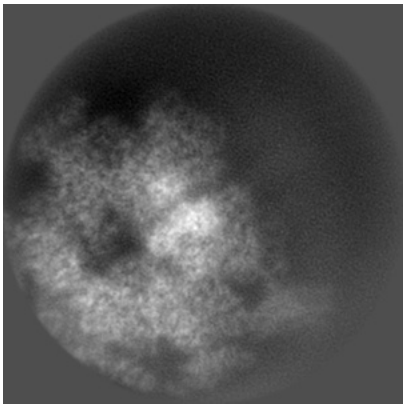


Z

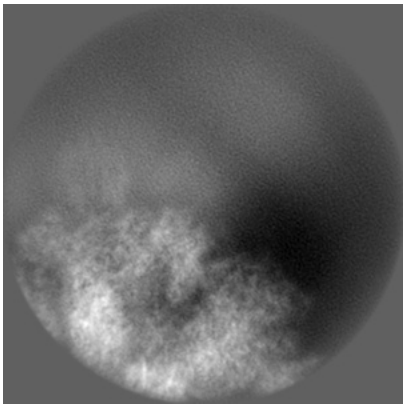
6.1.2 Raw map



X



Y

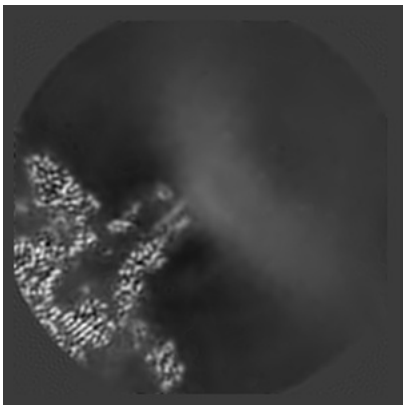


Z

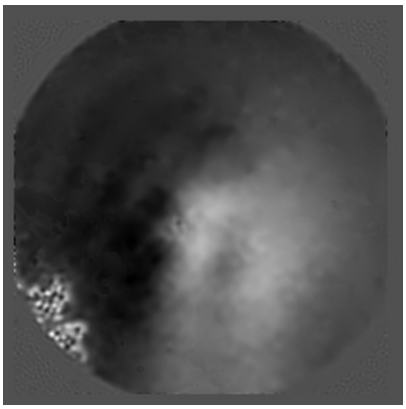
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

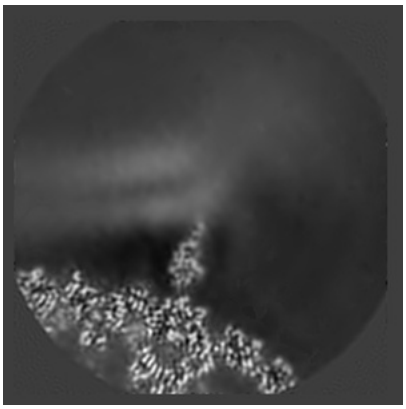
6.2.1 Primary map



X Index: 128

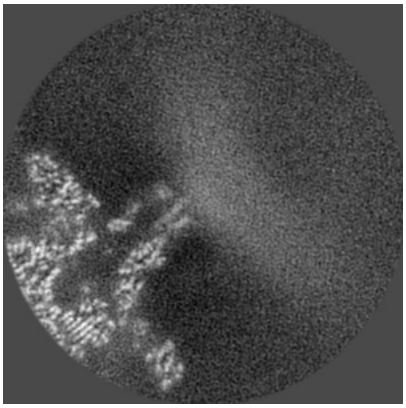


Y Index: 128

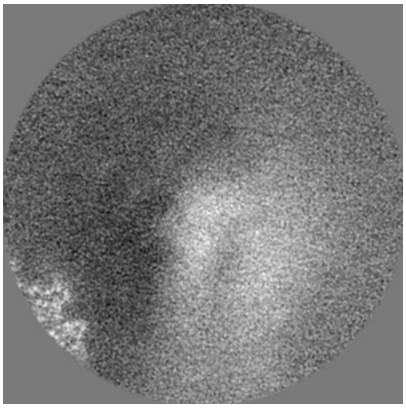


Z Index: 128

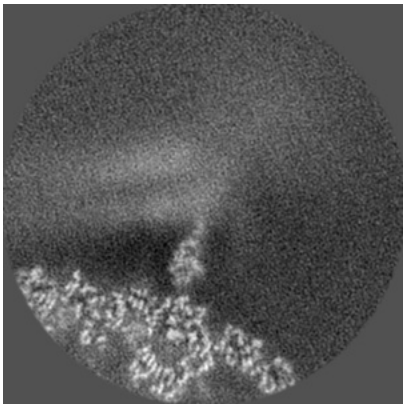
6.2.2 Raw map



X Index: 128



Y Index: 128

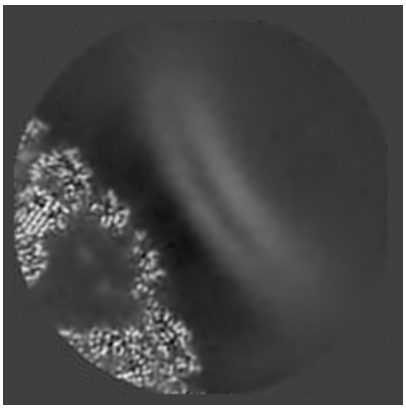


Z Index: 128

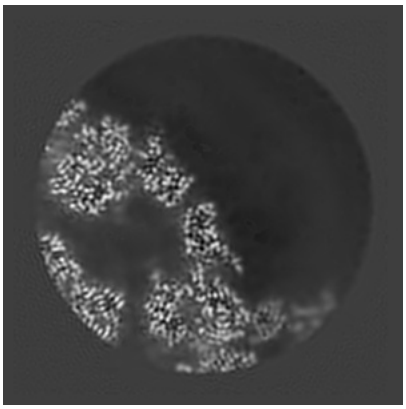
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

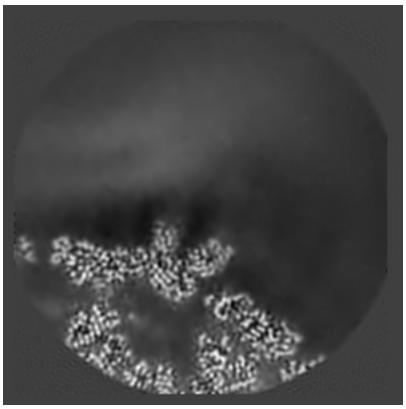
6.3.1 Primary map



X Index: 90

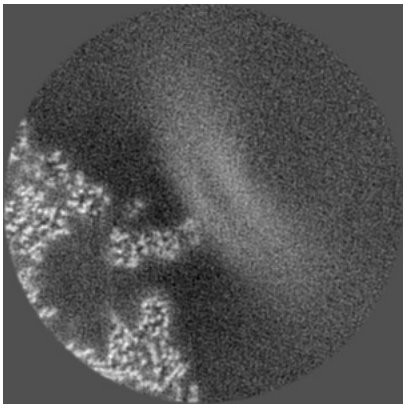


Y Index: 56

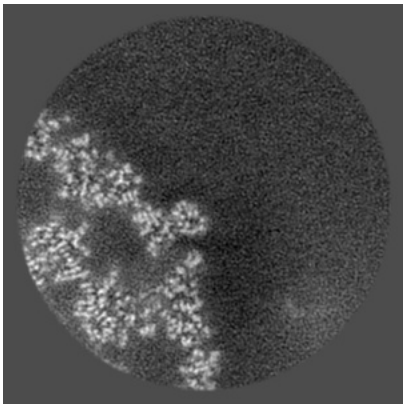


Z Index: 96

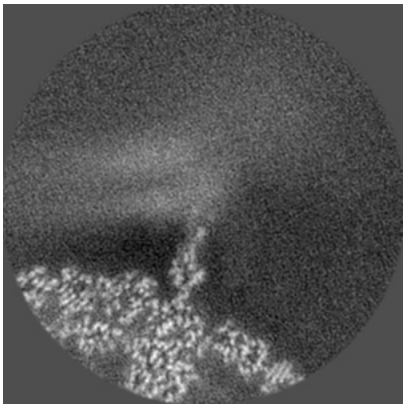
6.3.2 Raw map



X Index: 107



Y Index: 78

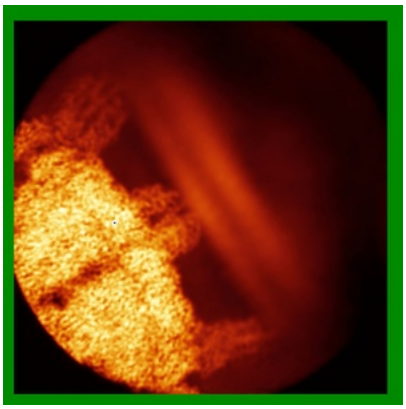


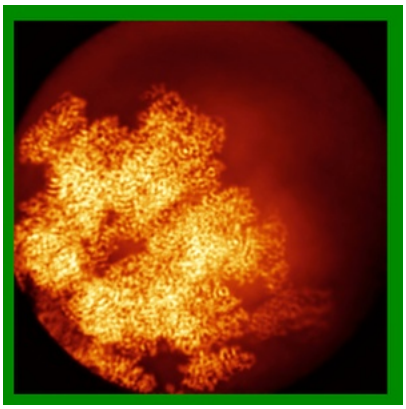
Z Index: 123

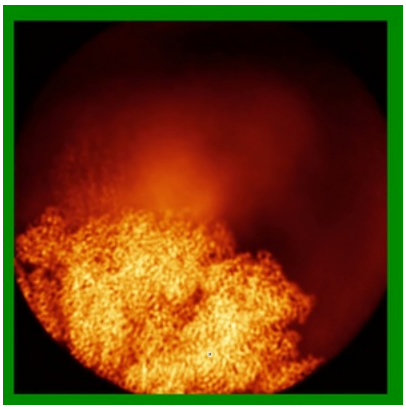
The images above show the largest variance slices of the map in three orthogonal directions.

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

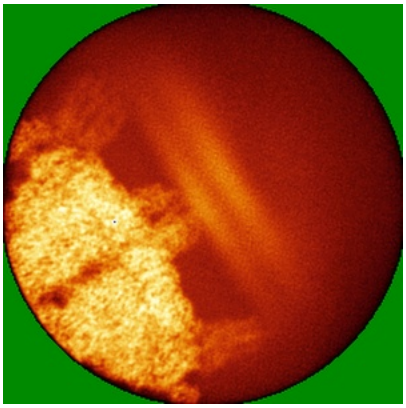
6.4.1 Primary map

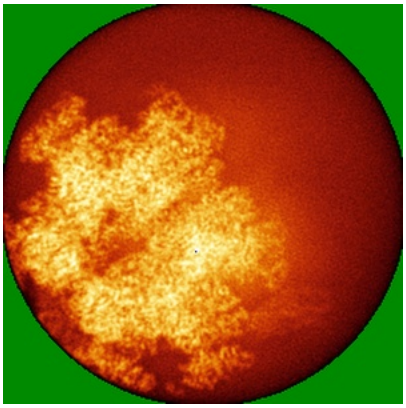

X

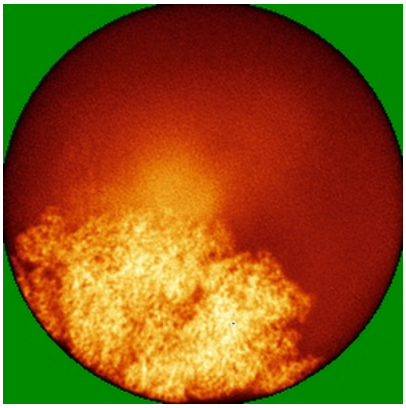

Y


Z

6.4.2 Raw map


X


Y

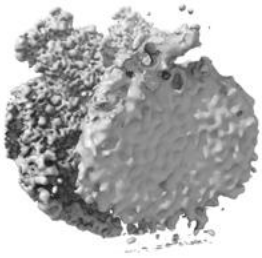

Z

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.

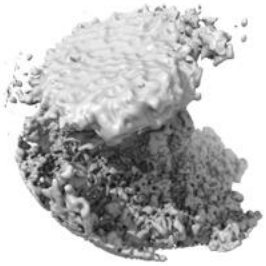
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



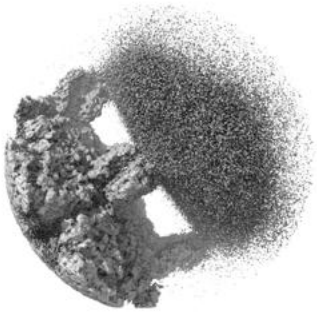
Y



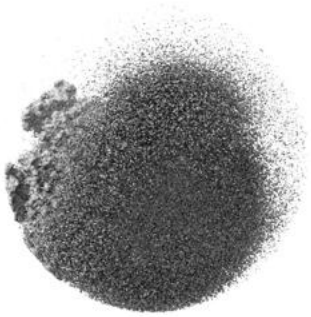
Z

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.

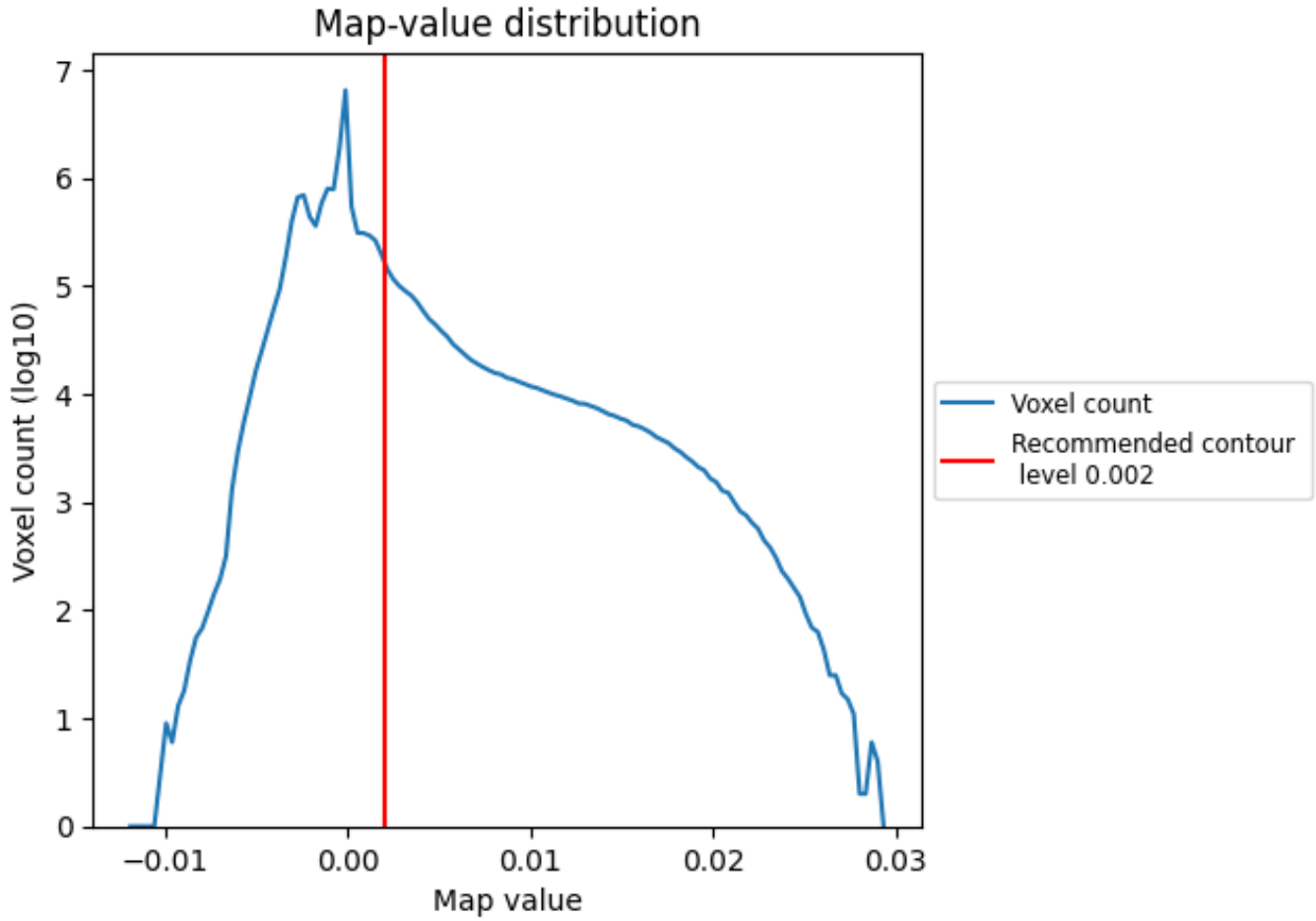
6.6 Mask visualisation (i)

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

7 Map analysis

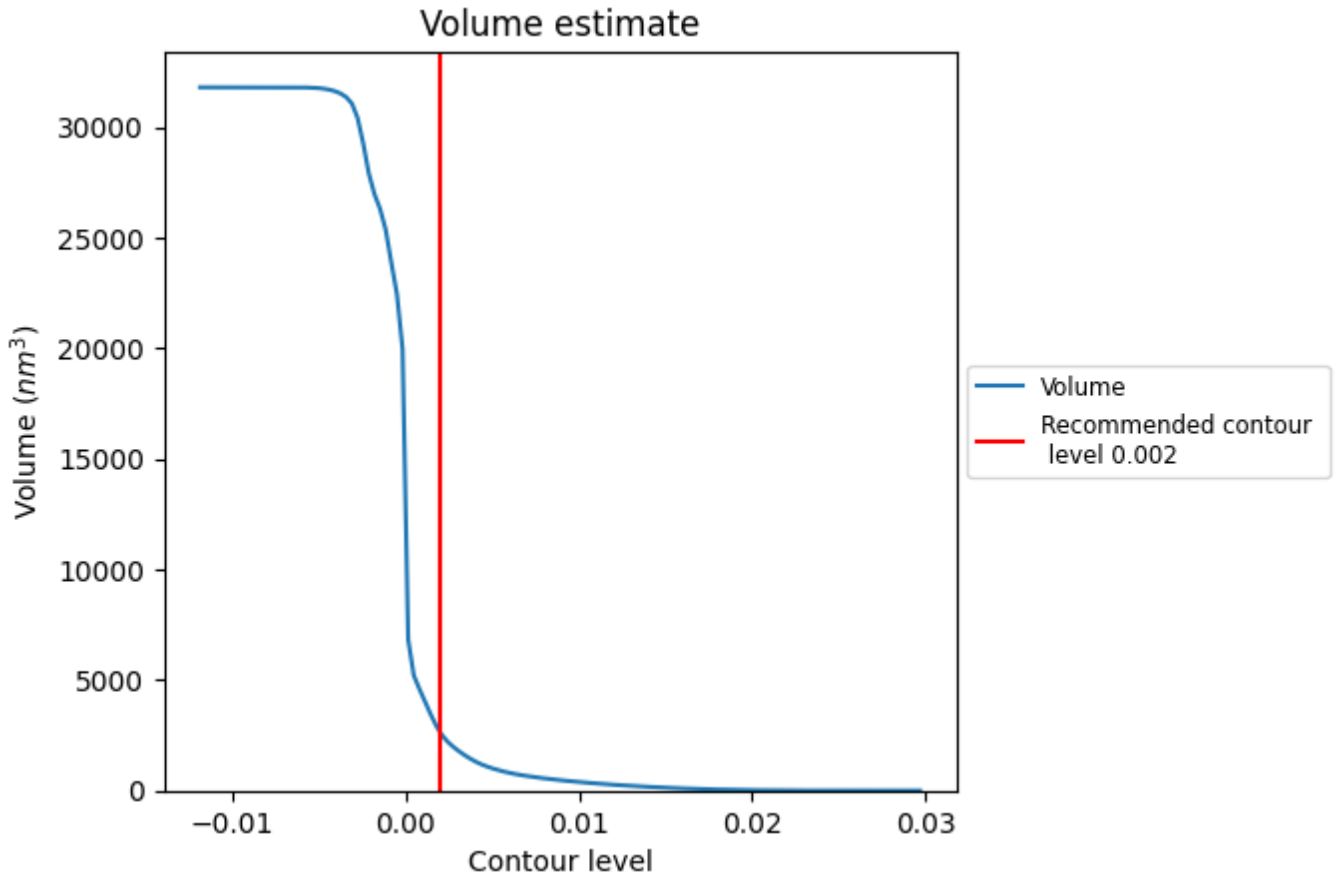
This section contains the results of statistical analysis of the map.

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.

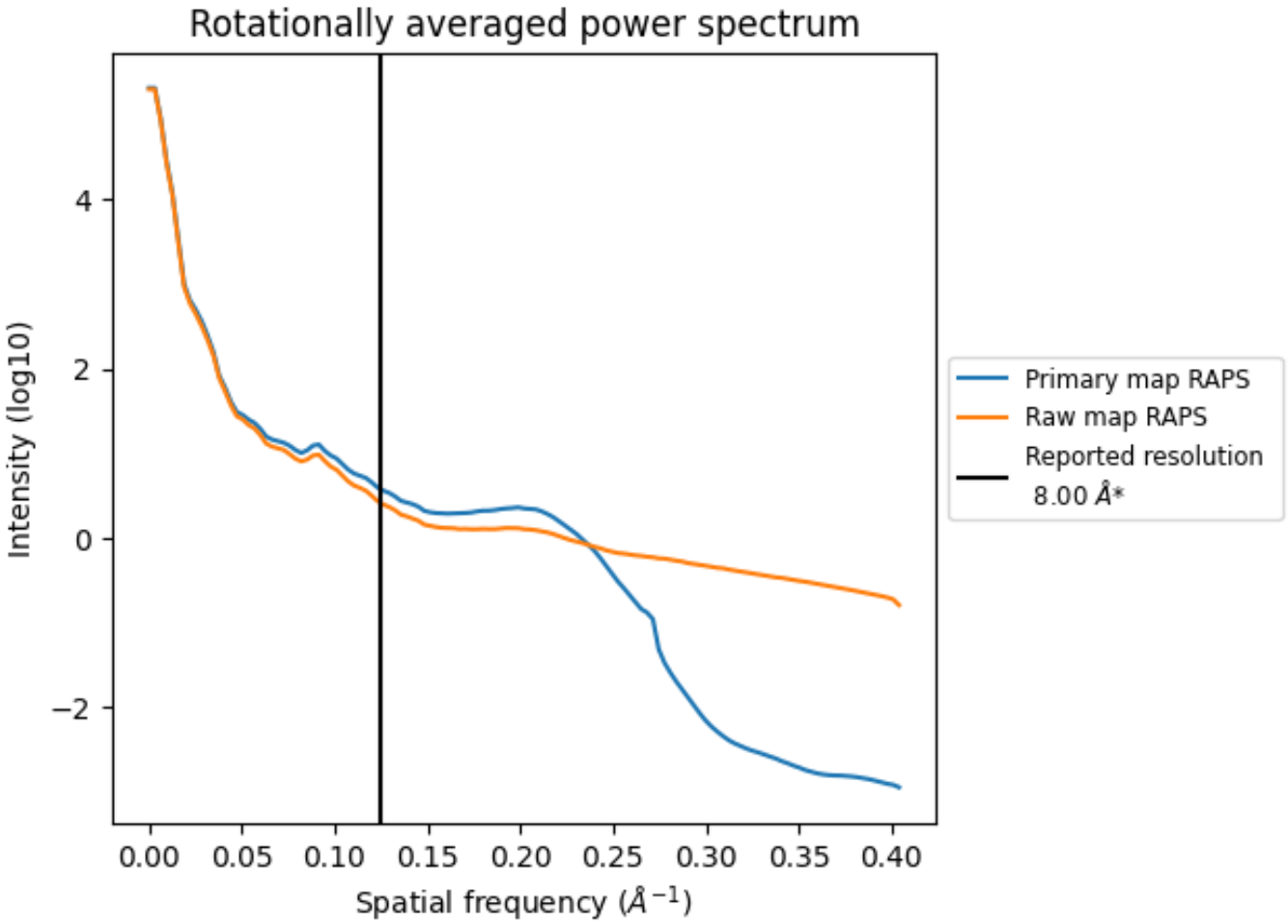
7.2 Volume estimate



The volume at the recommended contour level is 2619 nm^3; this corresponds to an approximate mass of 2366 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)

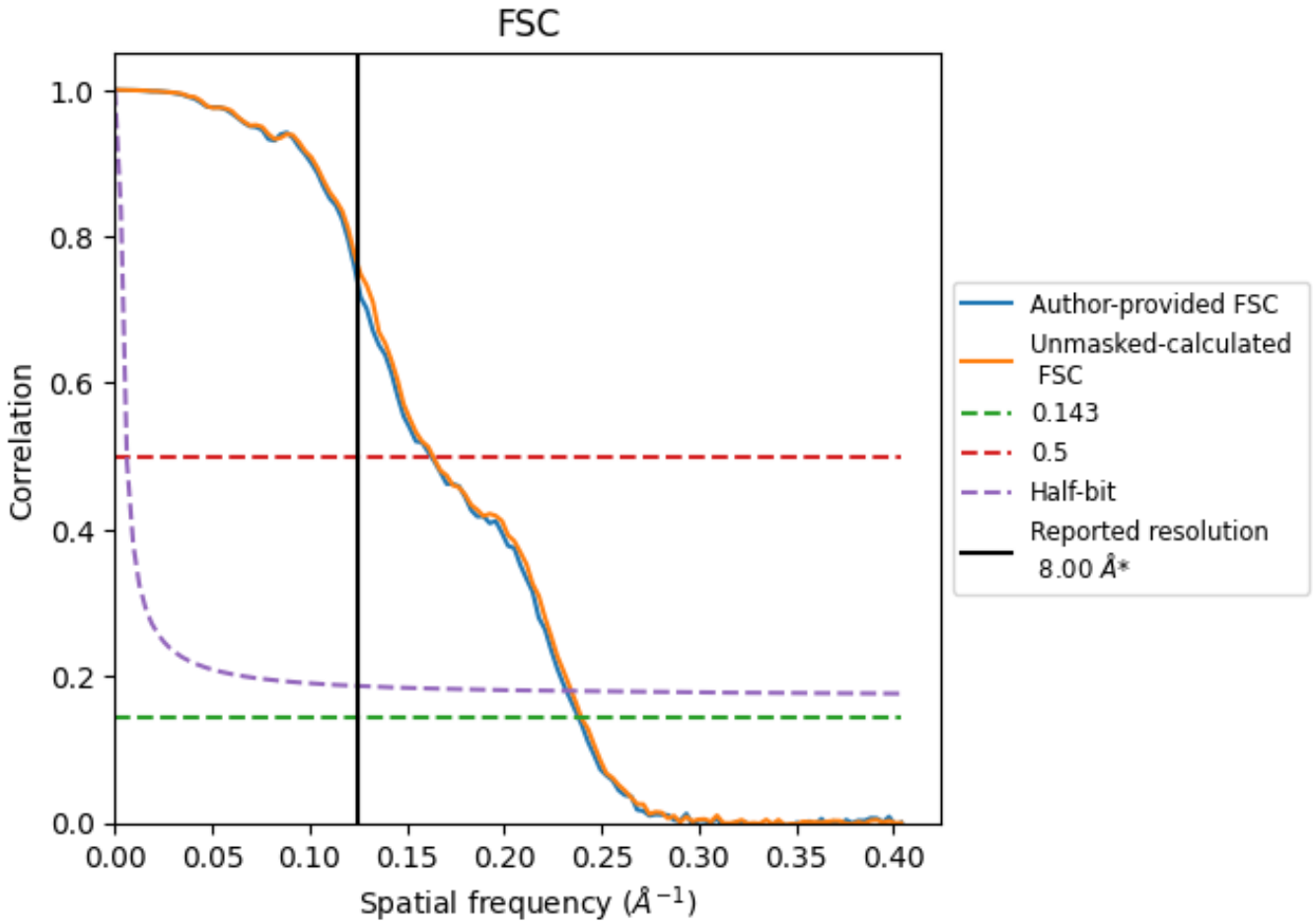


*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

8.2 Resolution estimates (i)

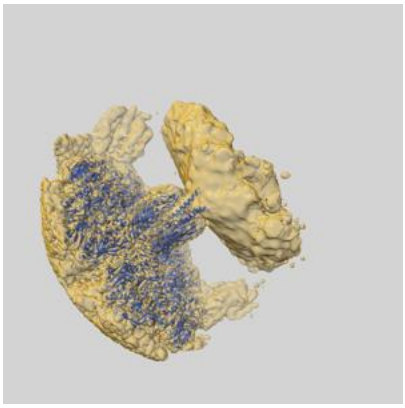
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	8.00
Author-provided FSC curve	4.20	6.15	4.31	-
Unmasked-calculated*	4.17	6.12	4.26	-

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

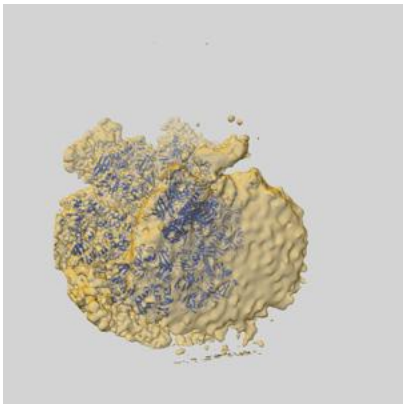
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42344 and PDB model 8UK3. Per-residue inclusion information can be found in section 3 on page 8.

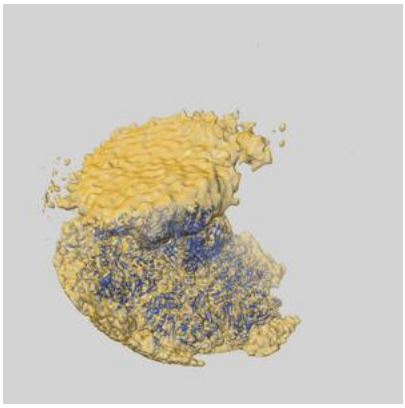
9.1 Map-model overlay



X



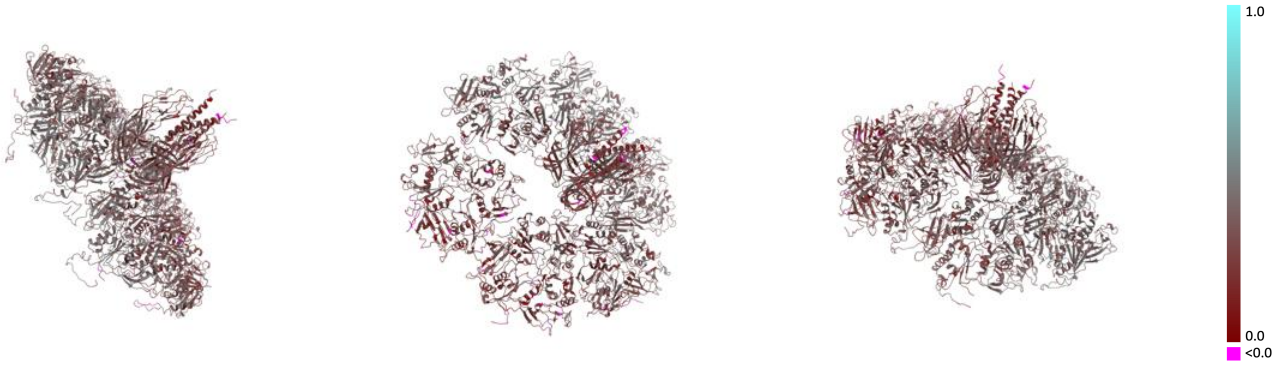
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.002 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.

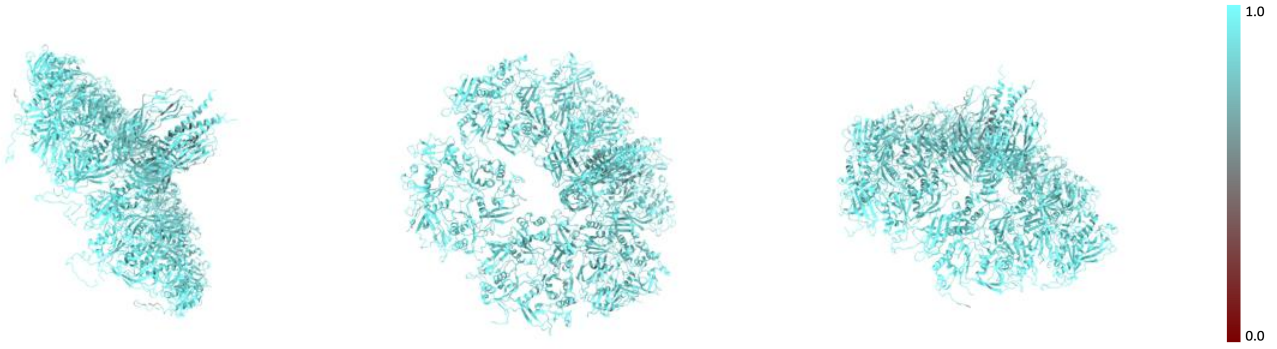
9.2 Q-score mapped to coordinate model (i)



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.

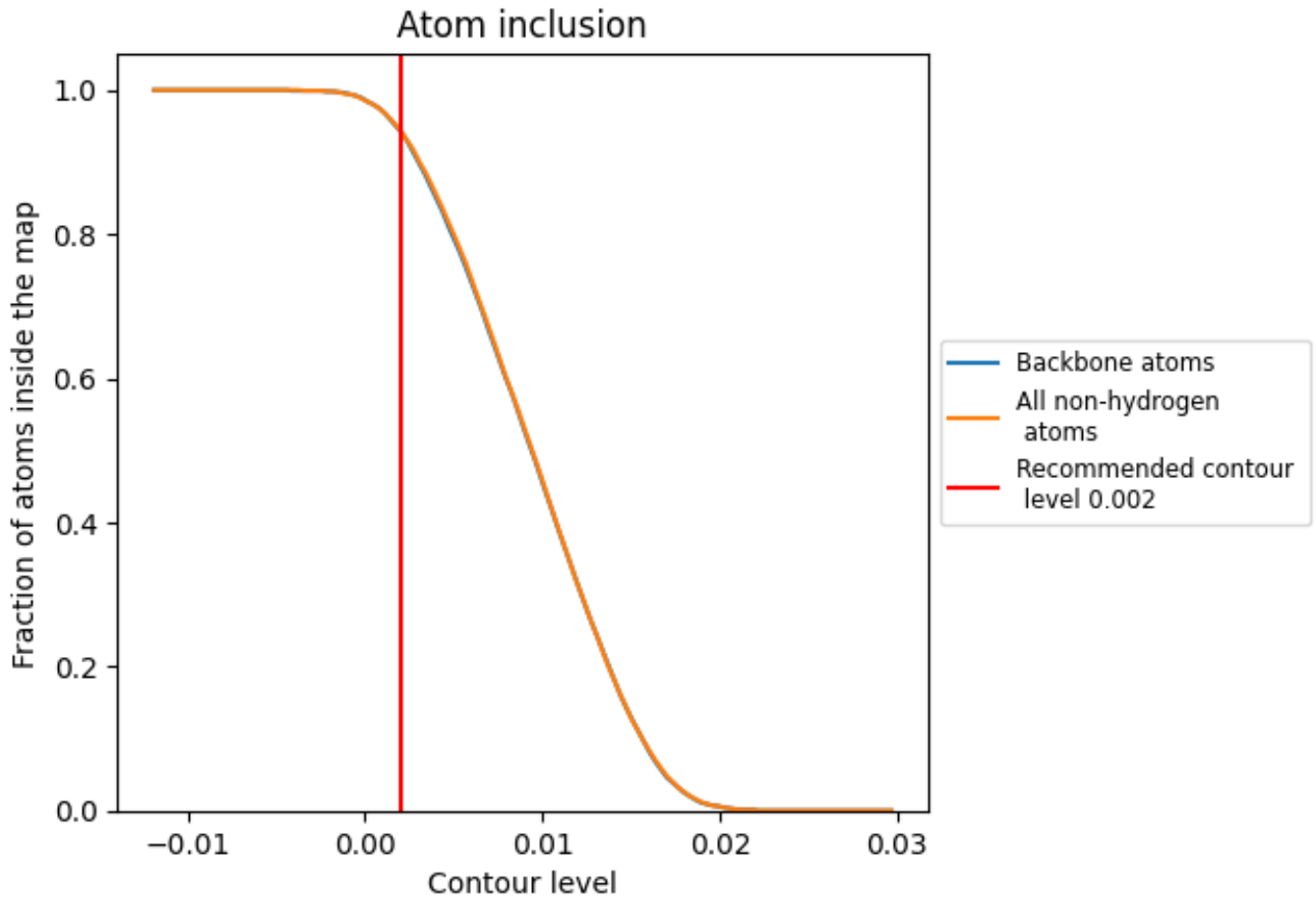
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.002).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% 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	0.9440	0.3270
1	0.8820	0.2730
2	0.9020	0.3010
3	0.9220	0.3000
a	0.9530	0.3470
b	0.9640	0.3730
c	0.9740	0.3810
d	0.9680	0.3880
e	0.9840	0.4030
f	0.9610	0.3890
g	0.9620	0.3430
h	0.9650	0.3470
i	0.9630	0.3760
j	0.9540	0.3020
k	0.9580	0.3380
l	0.9300	0.3100
m	0.9380	0.2890
n	0.9380	0.2860
o	0.9400	0.2520
p	0.9280	0.2680
q	0.9560	0.3310
r	0.9360	0.2660