



wwPDB EM Validation Summary Report ⓘ

Apr 23, 2025 – 11:36 PM EDT

PDB ID : 9C1J / pdb_00009c1j
EMDB ID : EMD-45121
Title : Rhesus rotavirus (reversed structure at 2.72 Angstrom resolution)
Authors : Jenni, S.; Herrmann, T.; De Sautu, M.; Harrison, S.C.
Deposited on : 2024-05-29
Resolution : 2.72 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev117
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) : 2.42

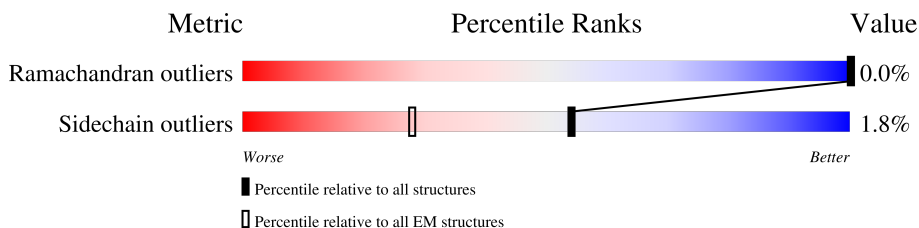
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.72 Å.

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









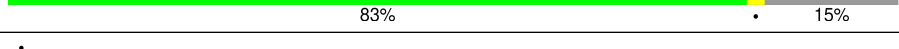
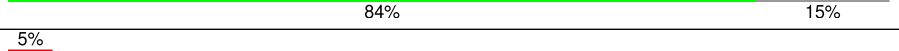
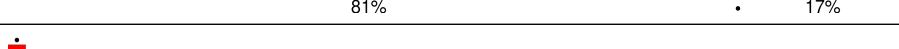
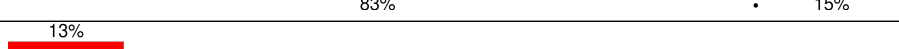


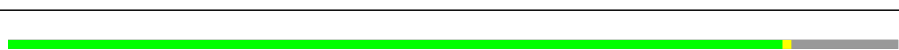

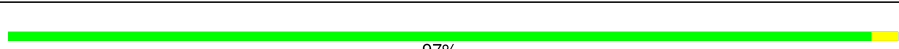
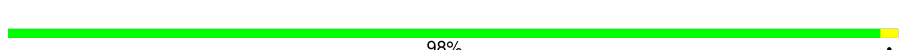

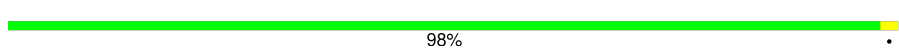
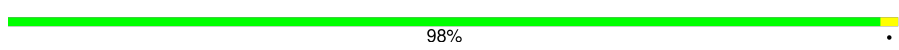
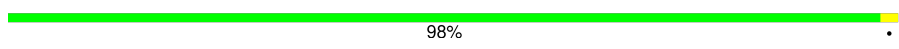
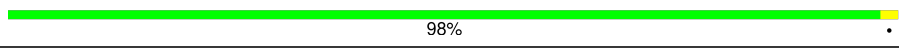
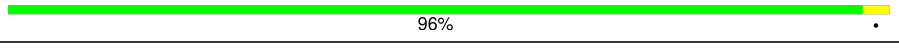
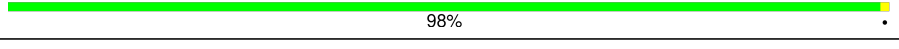
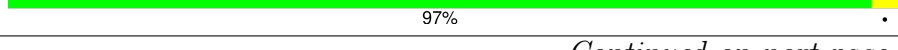

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	326	
1	1	326	
1	P	326	
1	Q	326	
1	R	326	
1	S	326	
1	T	326	
1	U	326	
1	V	326	

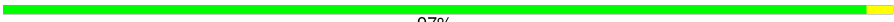








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Mol	Chain	Length	Quality of chain
1	W	326	
1	X	326	
1	Y	326	
1	Z	326	
1	t	326	
1	u	326	
1	v	326	
1	w	326	
1	x	326	
1	y	326	
2	2	776	
2	3	776	
2	4	776	
3	A	887	
3	B	887	
4	C	397	
4	D	397	
4	E	397	
4	F	397	
4	G	397	
4	H	397	
4	I	397	
4	J	397	
4	K	397	
4	L	397	

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Mol	Chain	Length	Quality of chain
4	M	397	 97% .
4	N	397	 96% .
4	O	397	 99% .
4	f	397	 98% .
4	g	397	 98% .
4	h	397	 97% .
4	i	397	 98% .
4	j	397	 97% .
4	k	397	 98% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 239272 atoms, of which 118354 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 glycoprotein VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	1	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	P	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	Q	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	R	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	S	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	T	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	U	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	V	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	W	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	X	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	Y	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	Z	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	t	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	u	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	v	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	w	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	x	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	y	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		

- Molecule 2 is a protein called Outer capsid protein VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		
2	3	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		
2	4	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	73	THR	SER	conflict	UNP P12473
2	311	GLU	ASP	conflict	UNP P12473
2	338	VAL	ILE	conflict	UNP P12473
2	421	LEU	PHE	conflict	UNP P12473
2	445	SER	GLY	conflict	UNP P12473
2	446	ARG	GLY	conflict	UNP P12473
2	454	ASN	TYR	conflict	UNP P12473
2	468	PHE	LEU	conflict	UNP P12473
2	519	ASP	TYR	conflict	UNP P12473
2	690	PHE	TYR	conflict	UNP P12473
3	73	THR	SER	conflict	UNP P12473
3	311	GLU	ASP	conflict	UNP P12473
3	338	VAL	ILE	conflict	UNP P12473
3	421	LEU	PHE	conflict	UNP P12473
3	445	SER	GLY	conflict	UNP P12473
3	446	ARG	GLY	conflict	UNP P12473
3	454	ASN	TYR	conflict	UNP P12473
3	468	PHE	LEU	conflict	UNP P12473
3	519	ASP	TYR	conflict	UNP P12473
3	690	PHE	TYR	conflict	UNP P12473
4	73	THR	SER	conflict	UNP P12473
4	311	GLU	ASP	conflict	UNP P12473
4	338	VAL	ILE	conflict	UNP P12473
4	421	LEU	PHE	conflict	UNP P12473

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Chain	Residue	Modelled	Actual	Comment	Reference
4	445	SER	GLY	conflict	UNP P12473
4	446	ARG	GLY	conflict	UNP P12473
4	454	ASN	TYR	conflict	UNP P12473
4	468	PHE	LEU	conflict	UNP P12473
4	519	ASP	TYR	conflict	UNP P12473
4	690	PHE	TYR	conflict	UNP P12473

- Molecule 3 is a protein called Inner capsid protein VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	779	Total	C	H	N	O	S	0	0
			12749	4041	6387	1098	1187	36		
3	B	799	Total	C	H	N	O	S	0	0
			13098	4154	6563	1126	1219	36		

- Molecule 4 is a protein called Intermediate capsid protein VP6.

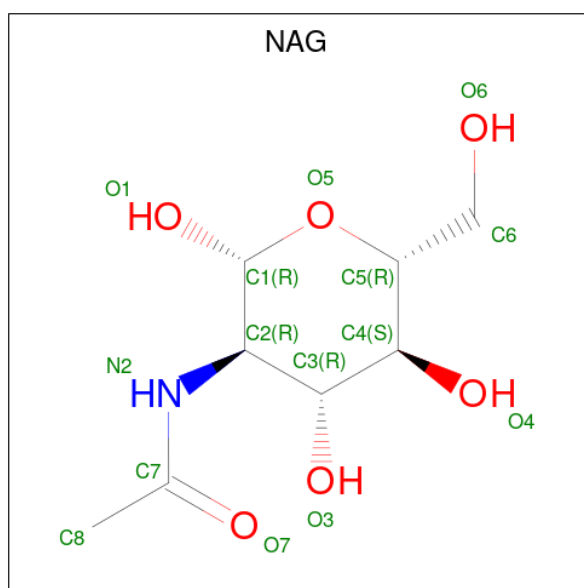
Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	397	Total	C	H	N	O	S	0	0
			6275	2005	3111	551	593	15		
4	D	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	E	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	F	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	G	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	H	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	I	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	J	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	K	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	L	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	M	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	N	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	O	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	f	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	g	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	h	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	i	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	j	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	k	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
5	0	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	1	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	P	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	Q	1	Total	C	H	N	O	0
			28	8	14	1	5	

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Mol	Chain	Residues	Atoms					AltConf
5	R	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	S	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	T	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	U	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	V	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	W	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	X	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	Y	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	Z	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	t	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	u	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	v	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	w	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	x	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	y	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	0	4	Total	Ca	0
			4	4	
6	1	4	Total	Ca	0
			4	4	
6	P	4	Total	Ca	0
			4	4	
6	Q	4	Total	Ca	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
6	R	4	Total 4	Ca 4	0
6	S	4	Total 4	Ca 4	0
6	T	4	Total 4	Ca 4	0
6	U	4	Total 4	Ca 4	0
6	V	4	Total 4	Ca 4	0
6	W	4	Total 4	Ca 4	0
6	X	4	Total 4	Ca 4	0
6	Y	4	Total 4	Ca 4	0
6	Z	4	Total 4	Ca 4	0
6	t	4	Total 4	Ca 4	0
6	u	4	Total 4	Ca 4	0
6	v	4	Total 4	Ca 4	0
6	w	4	Total 4	Ca 4	0
6	x	4	Total 4	Ca 4	0
6	y	4	Total 4	Ca 4	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	C	2	Total 2	Zn 2	0
7	D	1	Total 1	Zn 1	0
7	E	1	Total 1	Zn 1	0
7	F	2	Total 2	Zn 2	0

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Mol	Chain	Residues	Atoms		AltConf
7	G	1	Total 1	Zn 1	0
7	H	1	Total 1	Zn 1	0
7	I	2	Total 2	Zn 2	0
7	J	1	Total 1	Zn 1	0
7	K	1	Total 1	Zn 1	0
7	L	2	Total 2	Zn 2	0
7	M	1	Total 1	Zn 1	0
7	N	1	Total 1	Zn 1	0
7	O	2	Total 2	Zn 2	0
7	f	2	Total 2	Zn 2	0
7	g	1	Total 1	Zn 1	0
7	h	1	Total 1	Zn 1	0
7	i	2	Total 2	Zn 2	0
7	j	1	Total 1	Zn 1	0
7	k	1	Total 1	Zn 1	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
8	C	1	Total 1	Cl 1	0
8	F	1	Total 1	Cl 1	0
8	J	1	Total 1	Cl 1	0
8	M	1	Total 1	Cl 1	0

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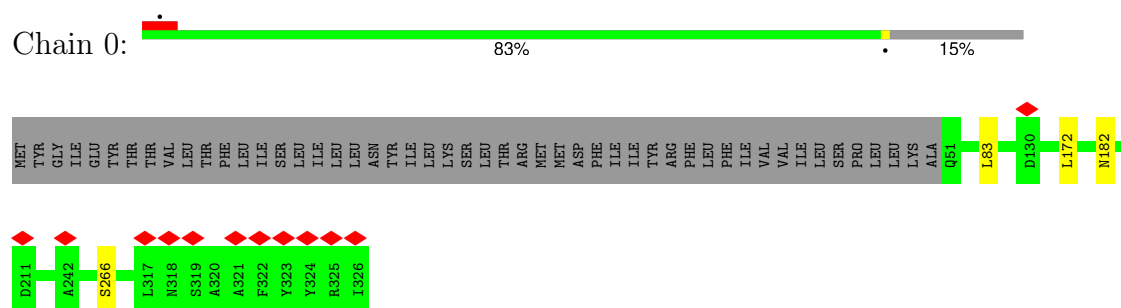
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Mol	Chain	Residues	Atoms		AltConf
8	O	1	Total 1	Cl 1	0
8	f	1	Total 1	Cl 1	0
8	j	1	Total 1	Cl 1	0

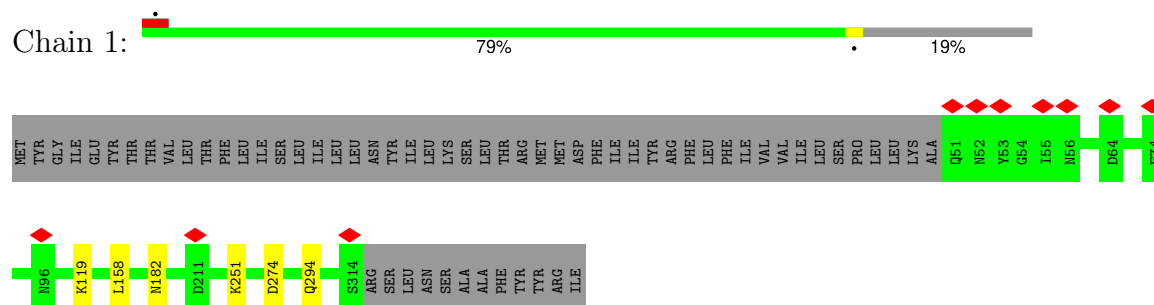
3 Residue-property plots [i](#)

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.

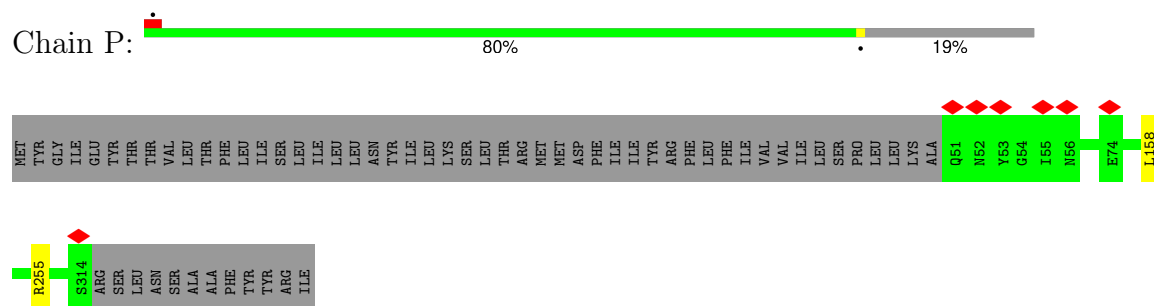
- Molecule 1: Outer capsid glycoprotein VP7



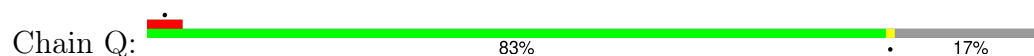
- Molecule 1: Outer capsid glycoprotein VP7

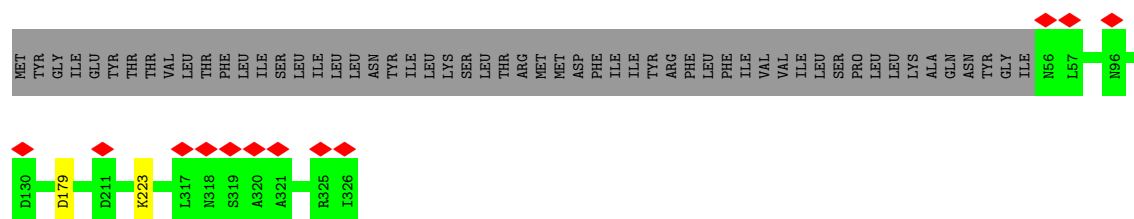


- Molecule 1: Outer capsid glycoprotein VP7



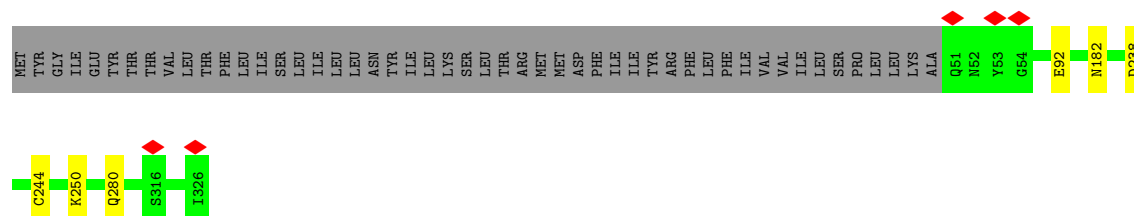
- Molecule 1: Outer capsid glycoprotein VP7





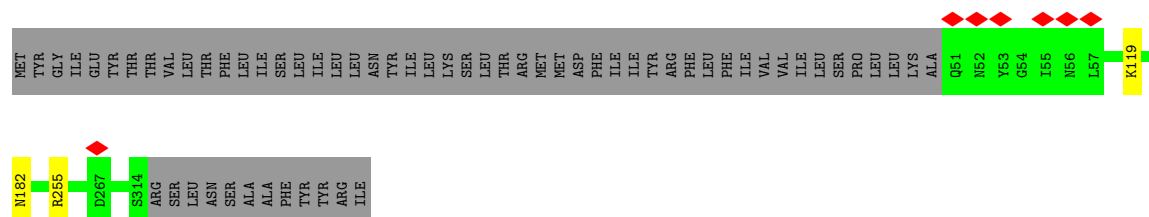
- Molecule 1: Outer capsid glycoprotein VP7

Chain R: 83% 15%



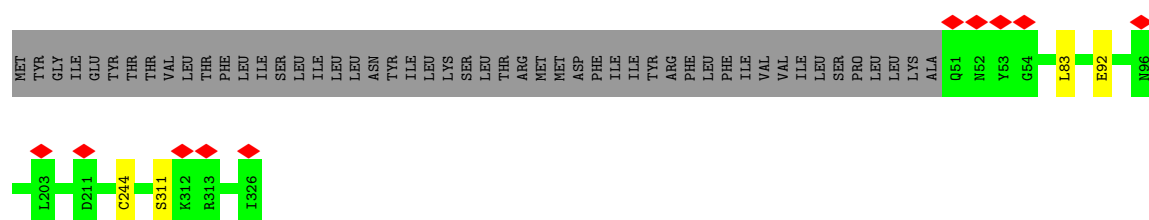
- Molecule 1: Outer capsid glycoprotein VP7

Chain S: 80% 19%



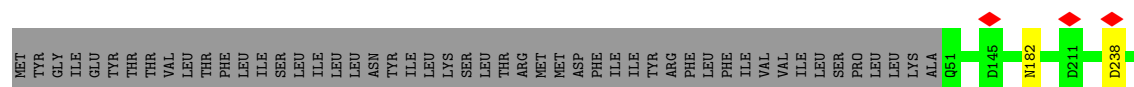
- Molecule 1: Outer capsid glycoprotein VP7

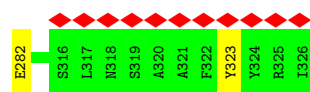
Chain T: 83% 15%



- Molecule 1: Outer capsid glycoprotein VP7

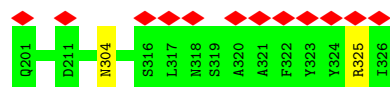
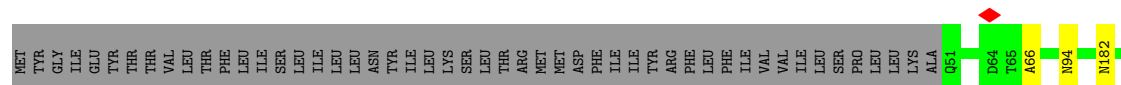
Chain U: 83% 15%





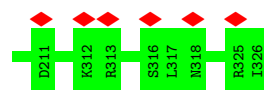
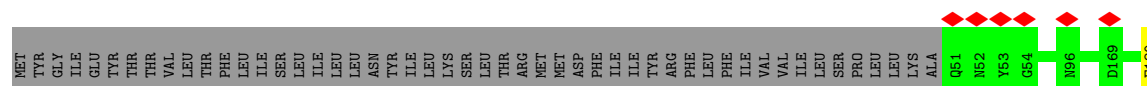
- Molecule 1: Outer capsid glycoprotein VP7

Chain V: 83% 15%



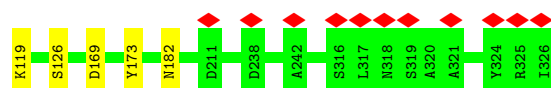
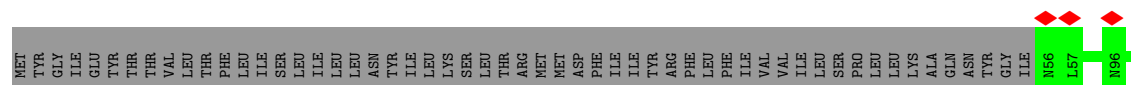
- Molecule 1: Outer capsid glycoprotein VP7

Chain W: 84% 15%



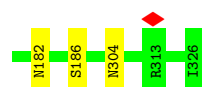
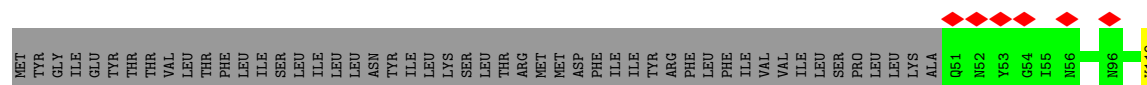
- Molecule 1: Outer capsid glycoprotein VP7

Chain X: 82% 17%




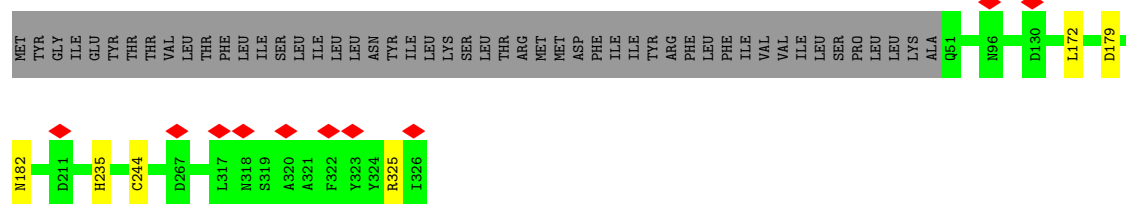
- Molecule 1: Outer capsid glycoprotein VP7

Chain Y: 83% 15%




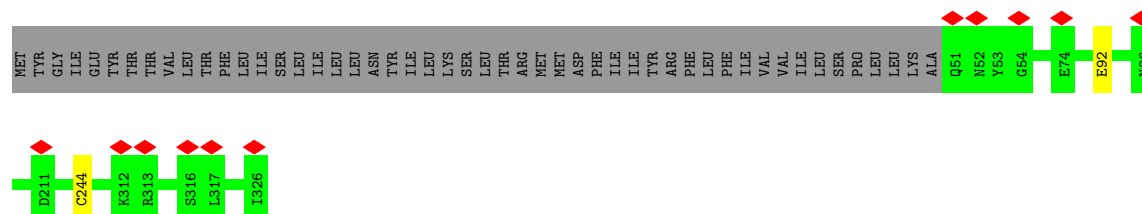
- Molecule 1: Outer capsid glycoprotein VP7

Chain Z:  83% 15%




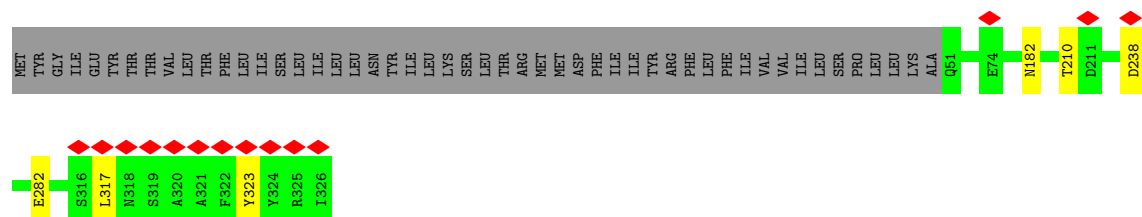
- Molecule 1: Outer capsid glycoprotein VP7

Chain t:  84% 15%




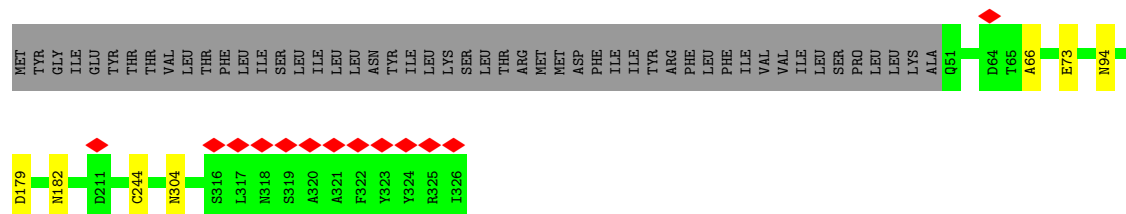
- Molecule 1: Outer capsid glycoprotein VP7

Chain u:  83% 15%




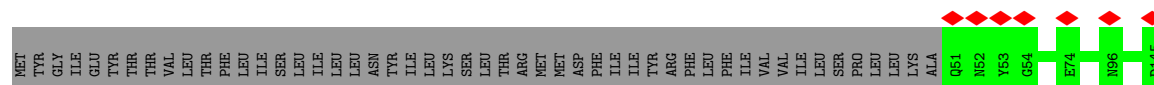
- Molecule 1: Outer capsid glycoprotein VP7

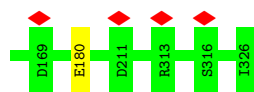
Chain v:  83% 15%



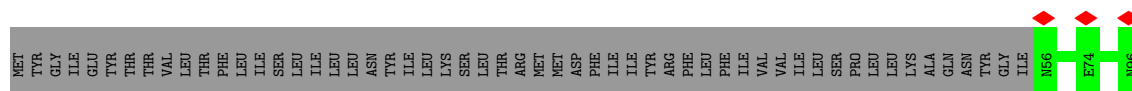
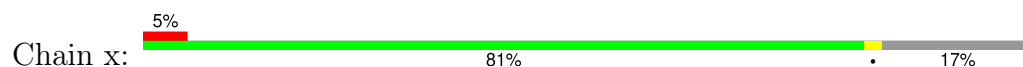
- Molecule 1: Outer capsid glycoprotein VP7

Chain w:  84% 15%

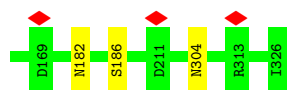
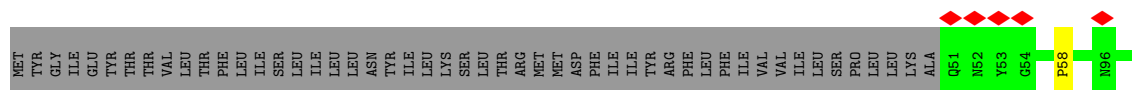
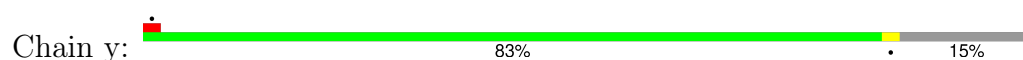




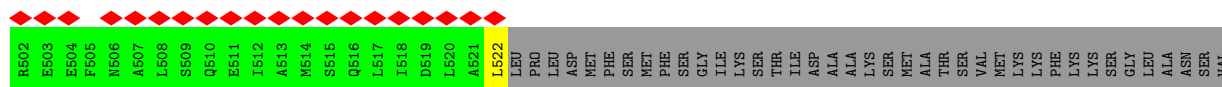
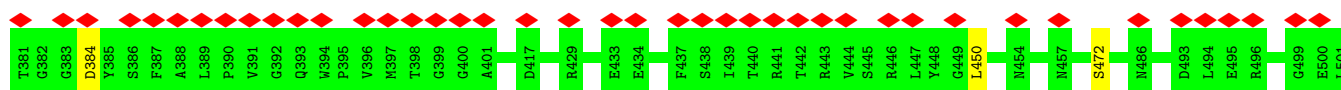
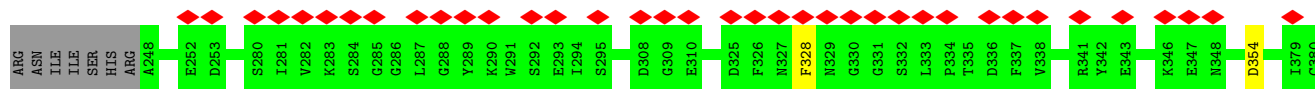
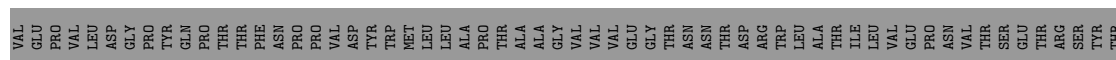
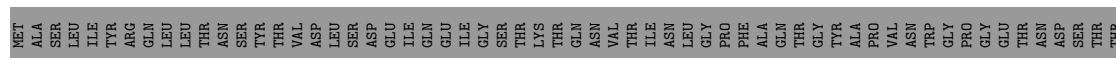
• Molecule 1: Outer capsid glycoprotein VP7



• Molecule 1: Outer capsid glycoprotein VP7



• Molecule 2: Outer capsid protein VP4



PHE	ASN	GLU	PHE	LYS	SER
LEU	LEU	ALA	GLU	GLU	THR
ARG	LEU	GLY	THR	ALA	THR
SER	SER	THR	GLN	ASP	ASP
ASP	ASP	GLY	THR	THR	LEU
PRO	PRO	ARG	GLU	GLU	SER
ARG	ARG	PHE	GLY	ASP	ASP
VAL	VAL	PHE	MET	ALA	ALA
LEU	LEU	ALA	ASN	ALA	ALA
ARG	ARG	TYR	PHE	SER	SER
GLU	GLU	ARG	ASP	ASP	SER
PHE	PHE	VAL	ASP	ILE	ILE
ILE	ILE	GLU	ILE	SER	SER
ASN	ASN	THR	SER	ARG	ARG
GLN	GLN	PHE	ALA	GLY	GLY
ASP	ASP	ASP	ALA	ALA	ALA
ASN	ASN	GLU	VAL	VAL	SER
PRO	PRO	ILE	LEU	LEU	ILE
ILE	ILE	PRO	LYS	LYS	ARG
ILE	ILE	PHE	THR	THR	SER
ARG	ARG	ASP	LYS	VAL	VAL
ASN	ASN	VAL	ILE	GLY	GLY
ARG	ARG	GLN	ASP	ASP	SER
LEU	LEU	LEU	THR	ALA	SER
ILE	ILE	LEU	ASP	GLN	ALA
MET	MET	VAL	LEU	ILE	TRP
GLN	GLN	THR	THR	SER	THR
CYS	CYS	ASP	PRO	ASP	THR
ARG	ARG	SER	SER	ASN	VAL
LEU	LEU	PRO	THR	SER	SER
		VAL	LEU	THR	THR
		ILE	PRO	GLN	GLN
		SER	ASP	ILE	ILE
		THR	VAL	THR	THR
		ALA	VAL	ASP	ASP
		ILE	THR	VAL	VAL
		ILE	GLU	SER	SER
		ASP	ALA	SER	SER
		PHE	LYS	VAL	VAL
		LEU	PHE	ILE	ILE
		LYS	ILE	ILE	ILE
		LEU	THR	SER	SER
		ASN	PRO	SER	SER
		LEU	ASN	THR	THR
		ASP	ARG	GLN	GLN
		THR	VAL	THR	THR
		GLY	ARG	THR	THR
		ILE	ILE	THR	THR
		SER	SER	THR	THR
		ARG	ASN	THR	THR
		GLN	ASN	GLN	GLN
		GLN	ASP	THR	THR
		GLN	GLU	ARG	ARG
		GLN	GLU	GLU	GLU

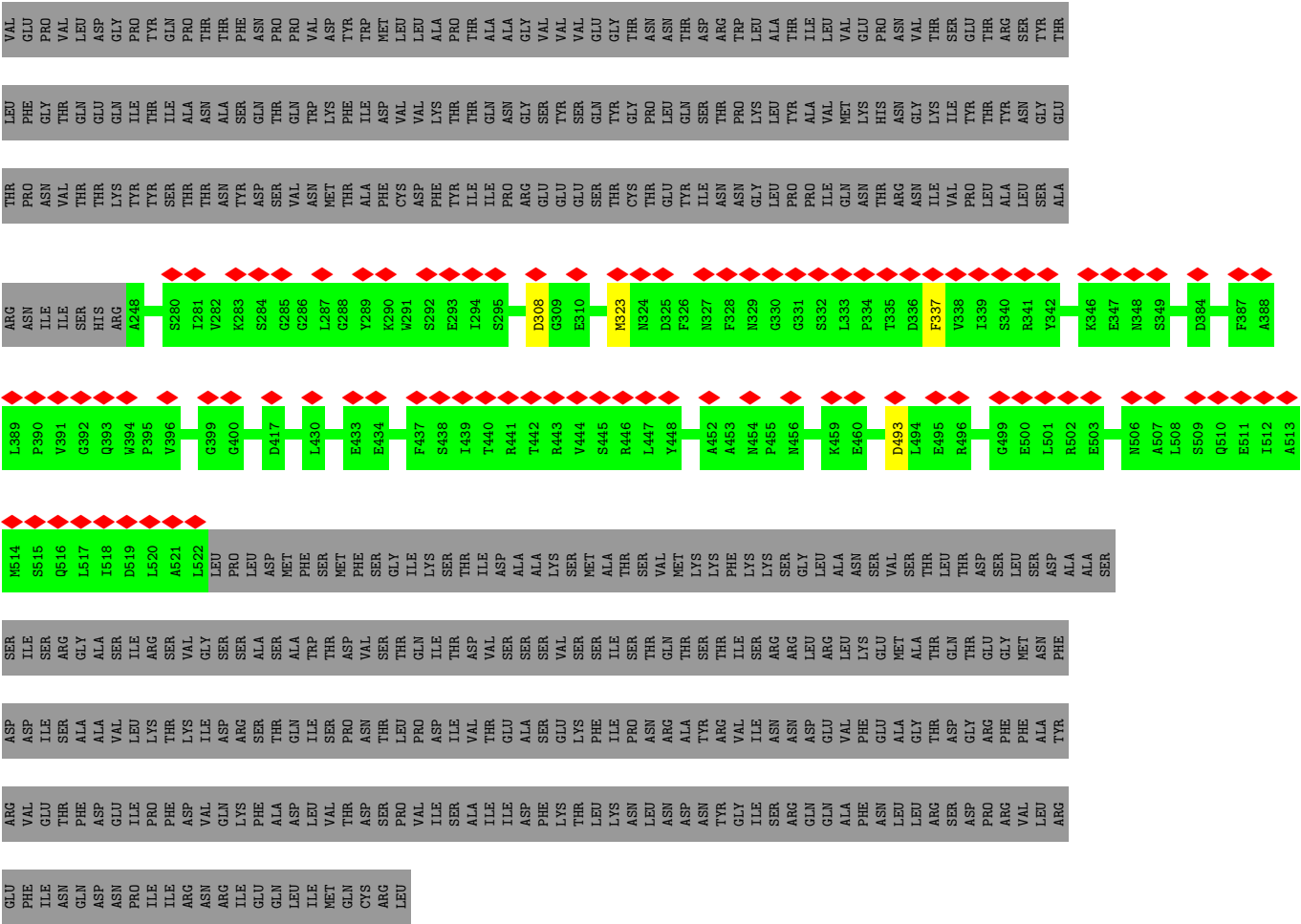
- Molecule 2: Outer capsid protein VP4

[illegible]

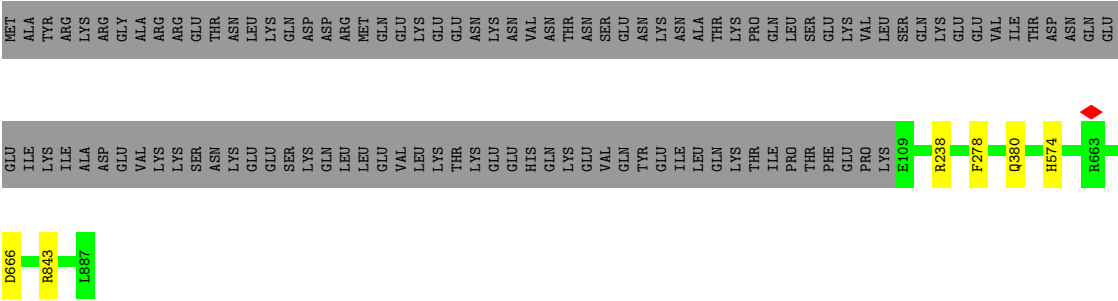
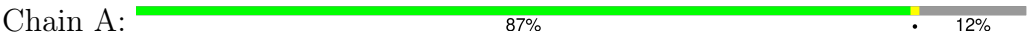
- Molecule 2: Outer capsid protein VP4



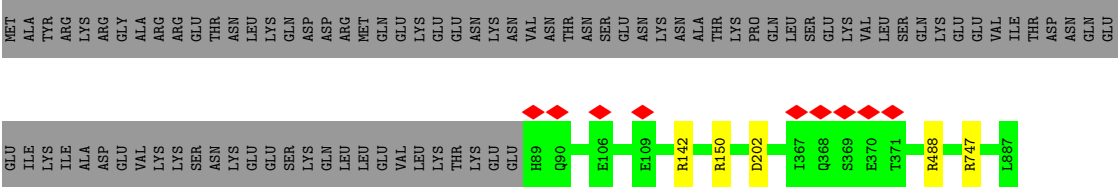
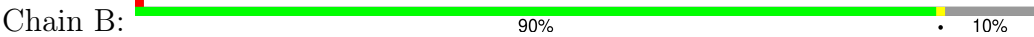
NET	ALA	SER	LEU	ILE	TYR	ARG	GLN	LEU	LEU	THR	ASN	SER	TYR	THR	VAL	ASP	LEU	SER	ASP	GLU	GLN	GLU	ILE	GLY	SER	THR	LYS	THR	GLN	ASN	VAL	THR	ILE	ASN	LEU	GLY	PRO	PHE	ALA	GLN	THR	GLY	TYR	ALA	PRO	VAL	ASN	TRP	GLY	PRO	GLY	GLU	THR	ASN	ASP	SER	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



● Molecule 3: Inner capsid protein VP2



● Molecule 3: Inner capsid protein VP2



- Molecule 4: Intermediate capsid protein VP6

Chain C:  97%



- Molecule 4: Intermediate capsid protein VP6

Chain D:  98%



- Molecule 4: Intermediate capsid protein VP6

Chain E:  97%



- Molecule 4: Intermediate capsid protein VP6

Chain F:  98%



- Molecule 4: Intermediate capsid protein VP6

Chain G:  98%



- Molecule 4: Intermediate capsid protein VP6

Chain H:  98%



- Molecule 4: Intermediate capsid protein VP6

Chain I:  98%



- Molecule 4: Intermediate capsid protein VP6

Chain J:  96%



- Molecule 4: Intermediate capsid protein VP6

Chain K:  98%



- Molecule 4: Intermediate capsid protein VP6

Chain L:  97%



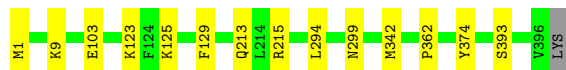
- Molecule 4: Intermediate capsid protein VP6

Chain M:  97%



- Molecule 4: Intermediate capsid protein VP6

Chain N:  96%



- Molecule 4: Intermediate capsid protein VP6

Chain O:  99%



- Molecule 4: Intermediate capsid protein VP6

Chain f:  98%



- Molecule 4: Intermediate capsid protein VP6

Chain g:  98% .



- Molecule 4: Intermediate capsid protein VP6

Chain h:  97% .



- Molecule 4: Intermediate capsid protein VP6

Chain i:  98% .



- Molecule 4: Intermediate capsid protein VP6

Chain j:  97% .



- Molecule 4: Intermediate capsid protein VP6

Chain k:  98% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1510279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.090	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	1267.2, 1267.2, 1267.2	wwPDB
Map dimensions	1536, 1536, 1536	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

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

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	0	0.25	0/2234	0.49	0/3051
1	1	0.25	0/2128	0.47	0/2908
1	P	0.25	0/2128	0.47	0/2908
1	Q	0.24	0/2192	0.48	0/2994
1	R	0.25	0/2234	0.48	0/3051
1	S	0.25	0/2128	0.47	0/2908
1	T	0.25	0/2234	0.48	0/3051
1	U	0.25	0/2234	0.49	0/3051
1	V	0.25	0/2234	0.50	0/3051
1	W	0.25	0/2234	0.47	0/3051
1	X	0.25	0/2192	0.47	0/2994
1	Y	0.25	0/2234	0.47	0/3051
1	Z	0.25	0/2234	0.49	0/3051
1	t	0.25	0/2234	0.48	0/3051
1	u	0.25	0/2234	0.49	0/3051
1	v	0.25	0/2234	0.48	0/3051
1	w	0.25	0/2234	0.47	0/3051
1	x	0.25	0/2192	0.47	0/2994
1	y	0.25	0/2234	0.48	0/3051
2	2	0.25	0/2232	0.51	0/3032
2	3	0.25	0/2232	0.51	0/3032
2	4	0.25	0/2232	0.51	0/3032
3	A	0.25	0/6477	0.50	0/8788
3	B	0.25	0/6655	0.49	0/9029
4	C	0.25	0/3224	0.52	0/4387
4	D	0.25	0/3215	0.53	0/4376
4	E	0.25	0/3215	0.52	0/4376
4	F	0.25	0/3215	0.53	0/4376
4	G	0.25	0/3215	0.52	0/4376
4	H	0.25	0/3215	0.52	0/4376
4	I	0.25	0/3215	0.52	0/4376
4	J	0.25	0/3215	0.53	0/4376

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	K	0.25	0/3215	0.51	0/4376
4	L	0.25	0/3215	0.52	0/4376
4	M	0.26	0/3215	0.52	0/4376
4	N	0.25	0/3215	0.53	0/4376
4	O	0.25	0/3215	0.53	0/4376
4	f	0.25	0/3215	0.53	0/4376
4	g	0.25	0/3215	0.52	0/4376
4	h	0.25	0/3215	0.52	0/4376
4	i	0.25	0/3215	0.52	0/4376
4	j	0.25	0/3215	0.53	0/4376
4	k	0.25	0/3215	0.52	0/4376
All	All	0.25	0/122924	0.50	0/167437

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	274/326 (84%)	266 (97%)	8 (3%)	0	100	100
1	1	262/326 (80%)	255 (97%)	7 (3%)	0	100	100
1	P	262/326 (80%)	259 (99%)	3 (1%)	0	100	100
1	Q	269/326 (82%)	268 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	S	262/326 (80%)	257 (98%)	5 (2%)	0	100	100
1	T	274/326 (84%)	273 (100%)	1 (0%)	0	100	100
1	U	274/326 (84%)	264 (96%)	10 (4%)	0	100	100
1	V	274/326 (84%)	264 (96%)	9 (3%)	1 (0%)	30	53
1	W	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	X	269/326 (82%)	264 (98%)	5 (2%)	0	100	100
1	Y	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	Z	274/326 (84%)	263 (96%)	11 (4%)	0	100	100
1	t	274/326 (84%)	268 (98%)	6 (2%)	0	100	100
1	u	274/326 (84%)	265 (97%)	9 (3%)	0	100	100
1	v	274/326 (84%)	263 (96%)	10 (4%)	1 (0%)	30	53
1	w	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	x	269/326 (82%)	264 (98%)	5 (2%)	0	100	100
1	y	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
2	2	273/776 (35%)	265 (97%)	8 (3%)	0	100	100
2	3	273/776 (35%)	264 (97%)	9 (3%)	0	100	100
2	4	273/776 (35%)	265 (97%)	8 (3%)	0	100	100
3	A	777/887 (88%)	765 (98%)	12 (2%)	0	100	100
3	B	797/887 (90%)	787 (99%)	10 (1%)	0	100	100
4	C	395/397 (100%)	385 (98%)	10 (2%)	0	100	100
4	D	394/397 (99%)	385 (98%)	9 (2%)	0	100	100
4	E	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	F	394/397 (99%)	382 (97%)	12 (3%)	0	100	100
4	G	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
4	H	394/397 (99%)	386 (98%)	8 (2%)	0	100	100
4	I	394/397 (99%)	386 (98%)	8 (2%)	0	100	100
4	J	394/397 (99%)	382 (97%)	12 (3%)	0	100	100
4	K	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	L	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	M	394/397 (99%)	382 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	O	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	f	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	g	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
4	h	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
4	i	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	j	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	k	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
All	All	15035/17839 (84%)	14702 (98%)	331 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	v	66	ALA
1	V	66	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	247/295 (84%)	243 (98%)	4 (2%)	58	81
1	1	237/295 (80%)	231 (98%)	6 (2%)	42	70
1	P	237/295 (80%)	235 (99%)	2 (1%)	79	91
1	Q	243/295 (82%)	241 (99%)	2 (1%)	79	91
1	R	247/295 (84%)	241 (98%)	6 (2%)	44	71
1	S	237/295 (80%)	234 (99%)	3 (1%)	65	84
1	T	247/295 (84%)	243 (98%)	4 (2%)	58	81
1	U	247/295 (84%)	243 (98%)	4 (2%)	58	81
1	V	247/295 (84%)	243 (98%)	4 (2%)	58	81
1	W	247/295 (84%)	246 (100%)	1 (0%)	89	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	243/295 (82%)	238 (98%)	5 (2%)	48	75
1	Y	247/295 (84%)	243 (98%)	4 (2%)	58	81
1	Z	247/295 (84%)	241 (98%)	6 (2%)	44	71
1	t	247/295 (84%)	245 (99%)	2 (1%)	79	91
1	u	247/295 (84%)	241 (98%)	6 (2%)	44	71
1	v	247/295 (84%)	241 (98%)	6 (2%)	44	71
1	w	247/295 (84%)	246 (100%)	1 (0%)	89	96
1	x	243/295 (82%)	237 (98%)	6 (2%)	42	70
1	y	247/295 (84%)	242 (98%)	5 (2%)	50	76
2	2	241/688 (35%)	235 (98%)	6 (2%)	42	70
2	3	241/688 (35%)	239 (99%)	2 (1%)	79	91
2	4	241/688 (35%)	237 (98%)	4 (2%)	56	80
3	A	715/818 (87%)	709 (99%)	6 (1%)	79	91
3	B	735/818 (90%)	730 (99%)	5 (1%)	81	92
4	C	349/349 (100%)	340 (97%)	9 (3%)	41	69
4	D	348/349 (100%)	341 (98%)	7 (2%)	50	76
4	E	348/349 (100%)	340 (98%)	8 (2%)	45	73
4	F	348/349 (100%)	342 (98%)	6 (2%)	56	80
4	G	348/349 (100%)	342 (98%)	6 (2%)	56	80
4	H	348/349 (100%)	342 (98%)	6 (2%)	56	80
4	I	348/349 (100%)	342 (98%)	6 (2%)	56	80
4	J	348/349 (100%)	336 (97%)	12 (3%)	32	59
4	K	348/349 (100%)	344 (99%)	4 (1%)	70	87
4	L	348/349 (100%)	339 (97%)	9 (3%)	41	69
4	M	348/349 (100%)	337 (97%)	11 (3%)	34	62
4	N	348/349 (100%)	335 (96%)	13 (4%)	29	56
4	O	348/349 (100%)	345 (99%)	3 (1%)	75	89
4	f	348/349 (100%)	342 (98%)	6 (2%)	56	80
4	g	348/349 (100%)	341 (98%)	7 (2%)	50	76
4	h	348/349 (100%)	340 (98%)	8 (2%)	45	73
4	i	348/349 (100%)	341 (98%)	7 (2%)	50	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	j	348/349 (100%)	337 (97%)	11 (3%)	34	62
4	k	348/349 (100%)	343 (99%)	5 (1%)	62	83
All	All	13437/15936 (84%)	13193 (98%)	244 (2%)	54	78

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	374	TYR
1	u	210	THR
1	S	119	LYS
1	t	244	CYS
1	x	169	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	t	305	GLN
1	w	305	GLN
1	y	308	GLN
1	y	305	GLN
1	S	305	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

19 non-standard protein/DNA/RNA residues are modelled in this entry.

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
4	FME	I	1	4	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
4	FME	M	1	4	8,9,10	0.38	0	8,9,11	1.04	1 (12%)
4	FME	g	1	4	8,9,10	0.38	0	8,9,11	1.07	1 (12%)
4	FME	j	1	4	8,9,10	0.38	0	8,9,11	1.04	1 (12%)
4	FME	H	1	4	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
4	FME	D	1	4	8,9,10	0.38	0	8,9,11	1.05	1 (12%)
4	FME	k	1	4	8,9,10	0.38	0	8,9,11	1.09	1 (12%)
4	FME	E	1	4	8,9,10	0.38	0	8,9,11	1.08	1 (12%)
4	FME	F	1	4	8,9,10	0.37	0	8,9,11	1.04	1 (12%)
4	FME	h	1	4	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
4	FME	O	1	4	8,9,10	0.38	0	8,9,11	1.05	1 (12%)
4	FME	f	1	4	8,9,10	0.37	0	8,9,11	1.06	1 (12%)
4	FME	K	1	4	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
4	FME	N	1	4	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
4	FME	J	1	4	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
4	FME	C	1	4	8,9,10	0.38	0	8,9,11	1.07	1 (12%)
4	FME	L	1	4	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
4	FME	G	1	4	8,9,10	0.38	0	8,9,11	1.04	1 (12%)
4	FME	i	1	4	8,9,10	0.38	0	8,9,11	1.00	1 (12%)

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
4	FME	I	1	4	-	1/7/9/11	-
4	FME	M	1	4	-	1/7/9/11	-
4	FME	g	1	4	-	1/7/9/11	-
4	FME	j	1	4	-	1/7/9/11	-
4	FME	H	1	4	-	1/7/9/11	-
4	FME	D	1	4	-	1/7/9/11	-
4	FME	k	1	4	-	1/7/9/11	-
4	FME	E	1	4	-	1/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	h	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	f	1	4	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	K	1	4	-	1/7/9/11	-
4	FME	N	1	4	-	1/7/9/11	-
4	FME	J	1	4	-	1/7/9/11	-
4	FME	C	1	4	-	1/7/9/11	-
4	FME	L	1	4	-	1/7/9/11	-
4	FME	G	1	4	-	1/7/9/11	-
4	FME	i	1	4	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	k	1	FME	CA-N-CN	2.47	126.63	122.82
4	E	1	FME	CA-N-CN	2.40	126.51	122.82
4	C	1	FME	CA-N-CN	2.40	126.51	122.82
4	I	1	FME	CA-N-CN	2.38	126.49	122.82
4	g	1	FME	CA-N-CN	2.38	126.48	122.82

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	FME	O1-CN-N-CA
4	D	1	FME	O1-CN-N-CA
4	E	1	FME	O1-CN-N-CA
4	F	1	FME	O1-CN-N-CA
4	G	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 109 are monoatomic - leaving 19 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	$\# Z > 2$
5	NAG	y	401	1	14,14,15	0.70	0	17,19,21	0.91	0
5	NAG	u	401	1	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
5	NAG	x	401	1	14,14,15	0.71	0	17,19,21	0.84	0
5	NAG	S	401	1	14,14,15	0.69	0	17,19,21	0.95	0
5	NAG	Q	401	1	14,14,15	0.69	0	17,19,21	0.98	0
5	NAG	0	401	1	14,14,15	0.70	0	17,19,21	0.98	0
5	NAG	X	401	1	14,14,15	0.70	0	17,19,21	0.84	0
5	NAG	V	401	1	14,14,15	0.69	0	17,19,21	0.93	0
5	NAG	1	401	1	14,14,15	0.73	0	17,19,21	0.92	0
5	NAG	T	401	1	14,14,15	0.71	0	17,19,21	0.92	0
5	NAG	t	401	1	14,14,15	0.71	0	17,19,21	0.87	0
5	NAG	w	401	1	14,14,15	0.71	0	17,19,21	0.87	0
5	NAG	U	401	1	14,14,15	0.70	0	17,19,21	0.89	0
5	NAG	Y	401	1	14,14,15	0.70	0	17,19,21	0.94	0
5	NAG	P	401	1	14,14,15	0.70	0	17,19,21	0.84	0
5	NAG	W	401	1	14,14,15	0.71	0	17,19,21	0.88	0
5	NAG	Z	401	1	14,14,15	0.70	0	17,19,21	0.92	0
5	NAG	R	401	1	14,14,15	0.70	0	17,19,21	0.88	0
5	NAG	v	401	1	14,14,15	0.71	0	17,19,21	0.88	0

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
5	NAG	y	401	1	-	3/6/23/26	0/1/1/1
5	NAG	u	401	1	-	2/6/23/26	0/1/1/1
5	NAG	x	401	1	-	4/6/23/26	0/1/1/1
5	NAG	S	401	1	-	4/6/23/26	0/1/1/1
5	NAG	Q	401	1	-	2/6/23/26	0/1/1/1
5	NAG	0	401	1	-	2/6/23/26	0/1/1/1
5	NAG	X	401	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	V	401	1	-	4/6/23/26	0/1/1/1
5	NAG	1	401	1	-	2/6/23/26	0/1/1/1
5	NAG	T	401	1	-	4/6/23/26	0/1/1/1
5	NAG	t	401	1	-	2/6/23/26	0/1/1/1
5	NAG	w	401	1	-	2/6/23/26	0/1/1/1
5	NAG	U	401	1	-	4/6/23/26	0/1/1/1
5	NAG	Y	401	1	-	2/6/23/26	0/1/1/1
5	NAG	P	401	1	-	2/6/23/26	0/1/1/1
5	NAG	W	401	1	-	2/6/23/26	0/1/1/1
5	NAG	Z	401	1	-	3/6/23/26	0/1/1/1
5	NAG	R	401	1	-	4/6/23/26	0/1/1/1
5	NAG	v	401	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	u	401	NAG	O5-C1-C2	-2.06	108.11	111.29

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	v	401	NAG	O5-C5-C6-O6
5	T	401	NAG	O5-C5-C6-O6
5	R	401	NAG	O5-C5-C6-O6
5	v	401	NAG	C4-C5-C6-O6
5	T	401	NAG	C4-C5-C6-O6

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 ⓘ

There are no chain breaks in this entry.

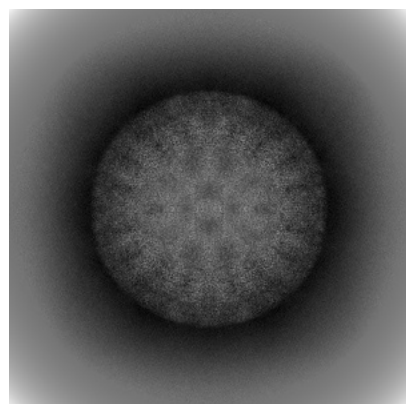
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45121. These allow visual inspection of the internal detail of the map and identification of artifacts.

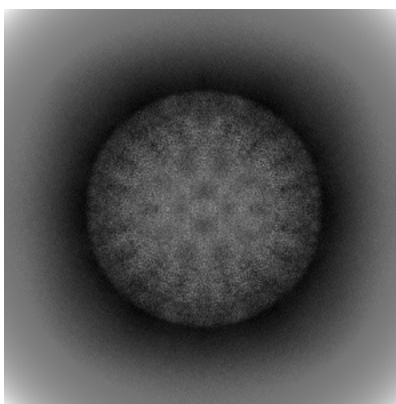
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

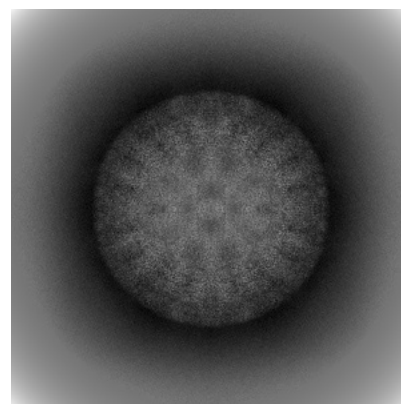
6.1.1 Primary map



X

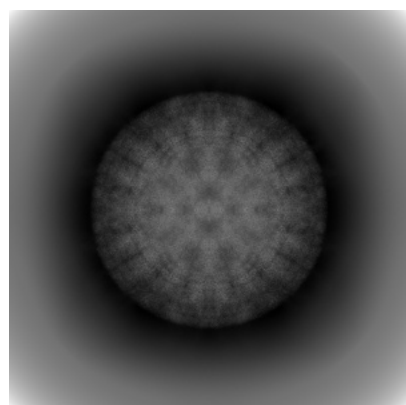


Y

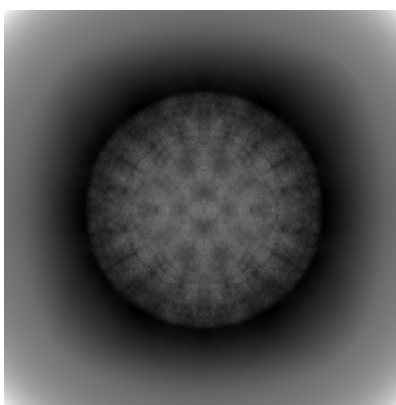


Z

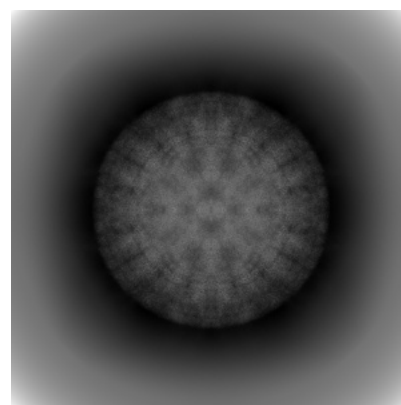
6.1.2 Raw map



X



Y

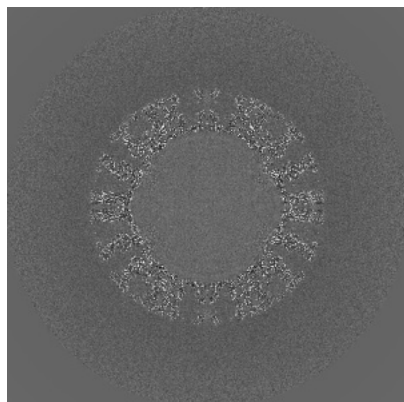


Z

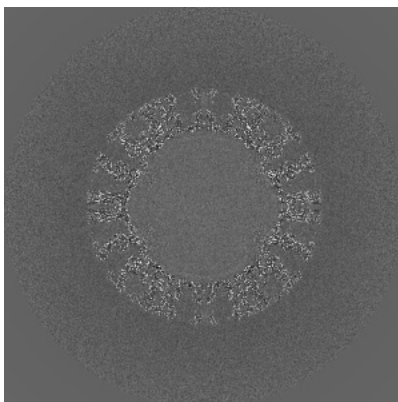
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

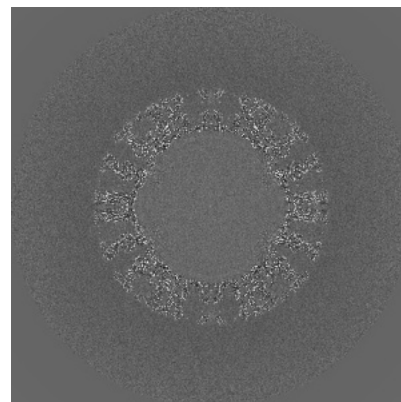
6.2.1 Primary map



X Index: 768

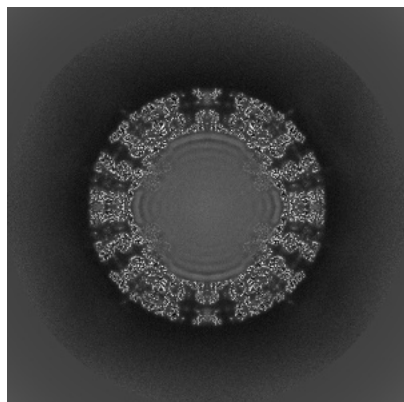


Y Index: 768

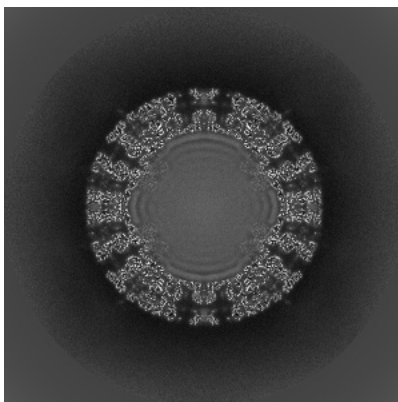


Z Index: 768

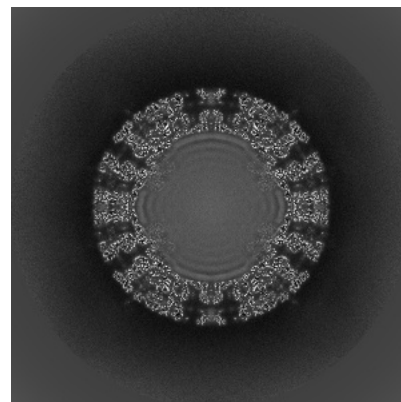
6.2.2 Raw map



X Index: 768



Y Index: 768

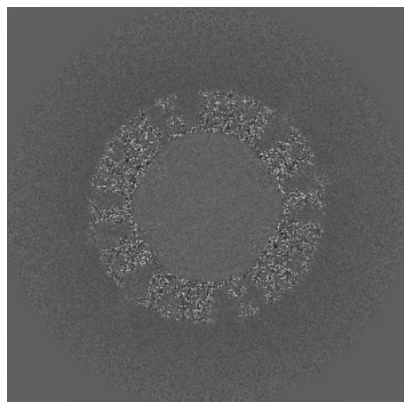


Z Index: 768

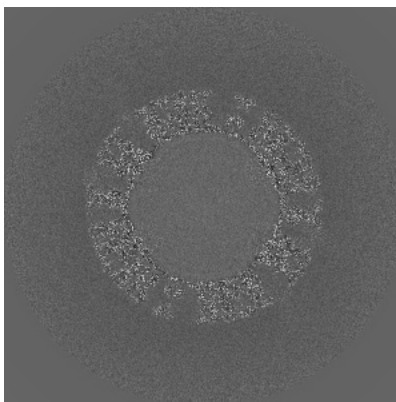
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

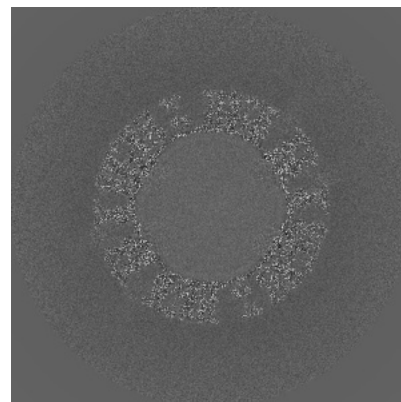
6.3.1 Primary map



X Index: 800

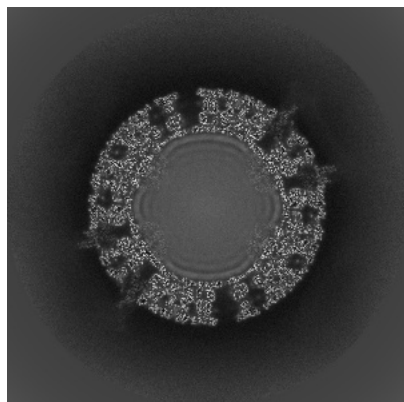


Y Index: 736

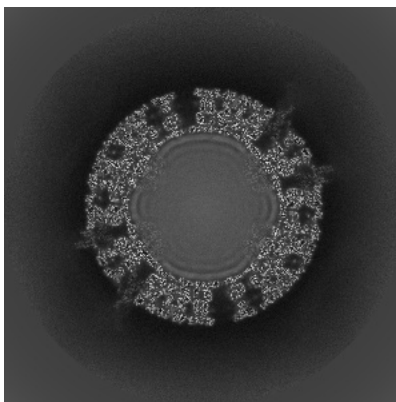


Z Index: 800

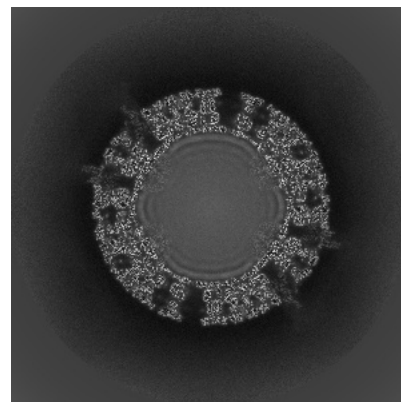
6.3.2 Raw map



X Index: 794



Y Index: 794

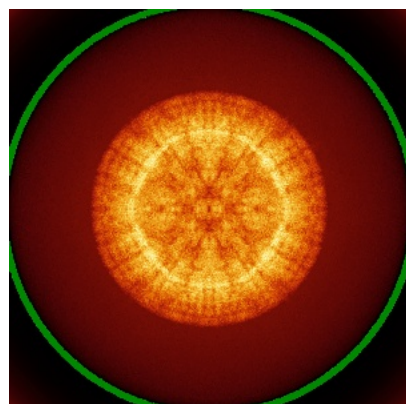


Z Index: 742

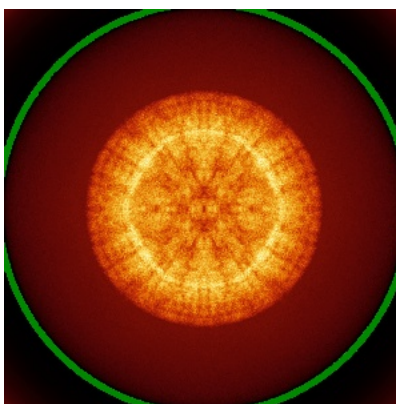
The images above show the largest variance slices of the map in three orthogonal directions.

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

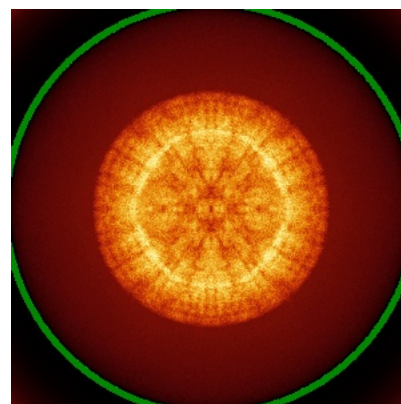
6.4.1 Primary map



X

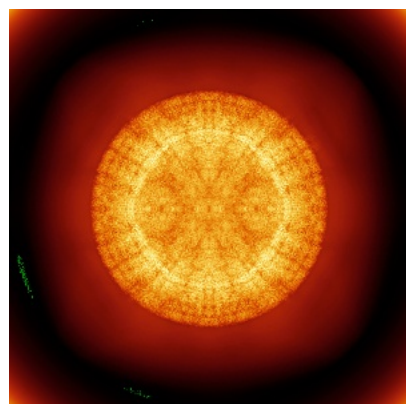


Y

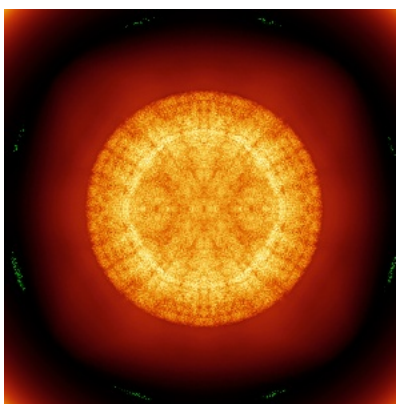


Z

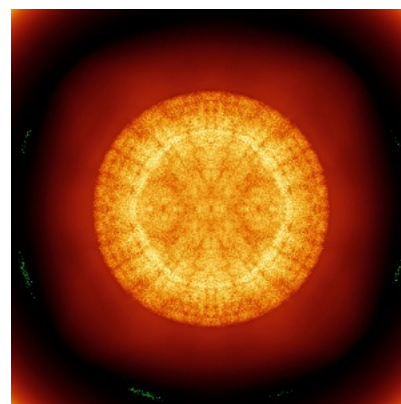
6.4.2 Raw map



X



Y

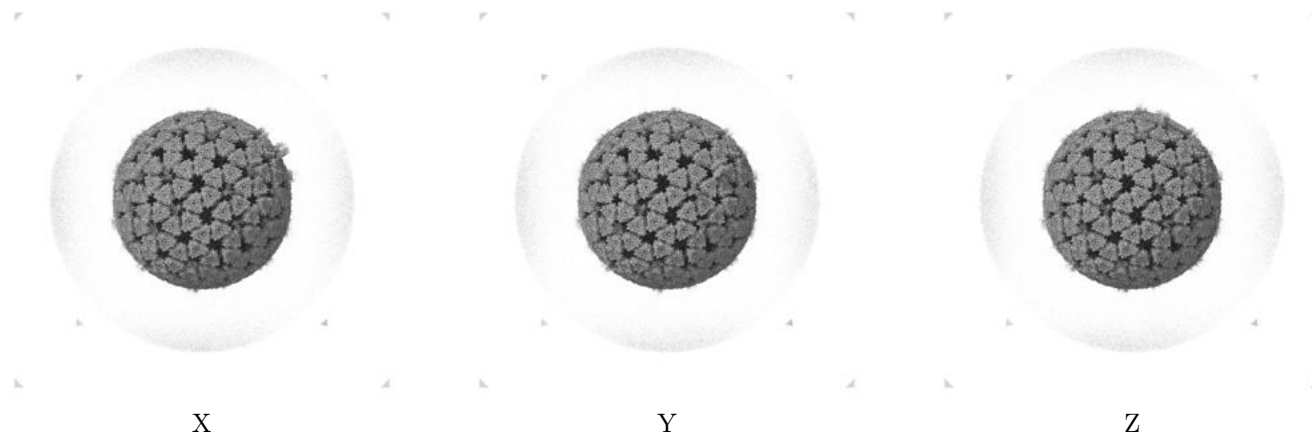


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

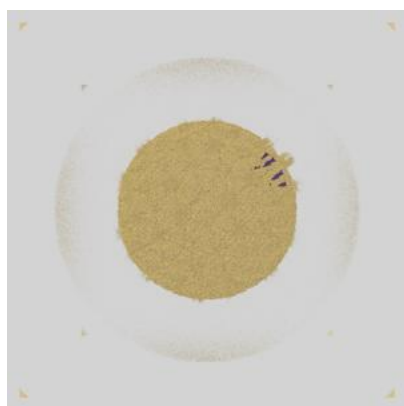
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

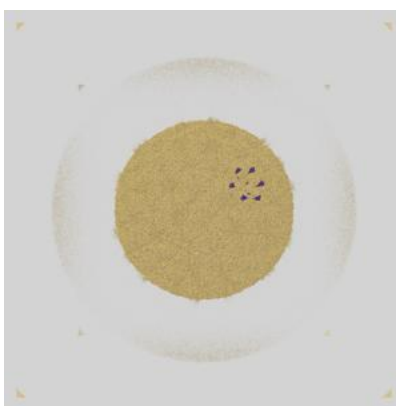
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

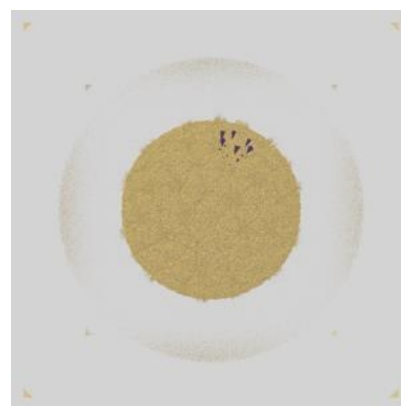
6.6.1 emd_45121_msk_1.map [i](#)



X



Y

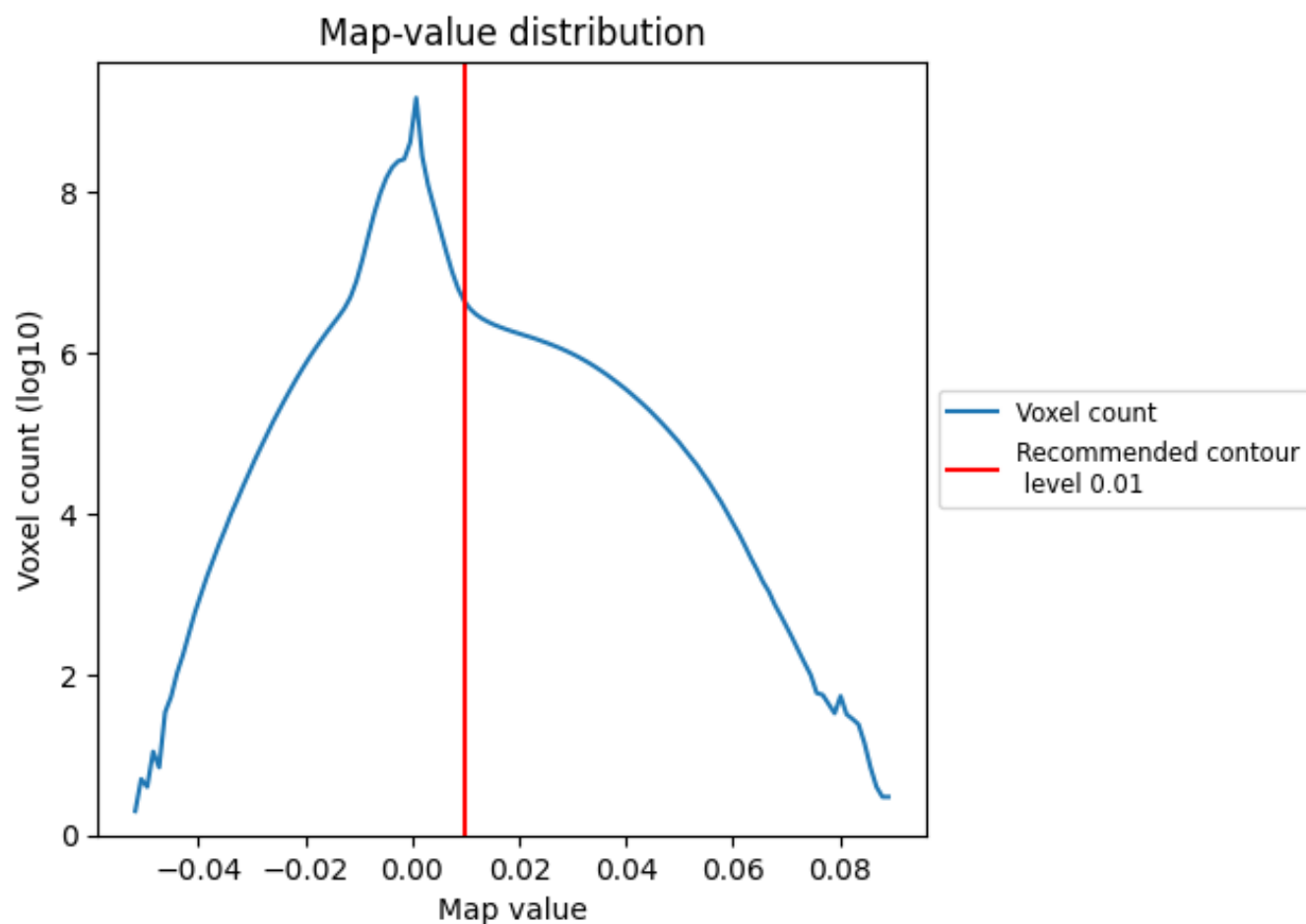


Z

7 Map analysis [i](#)

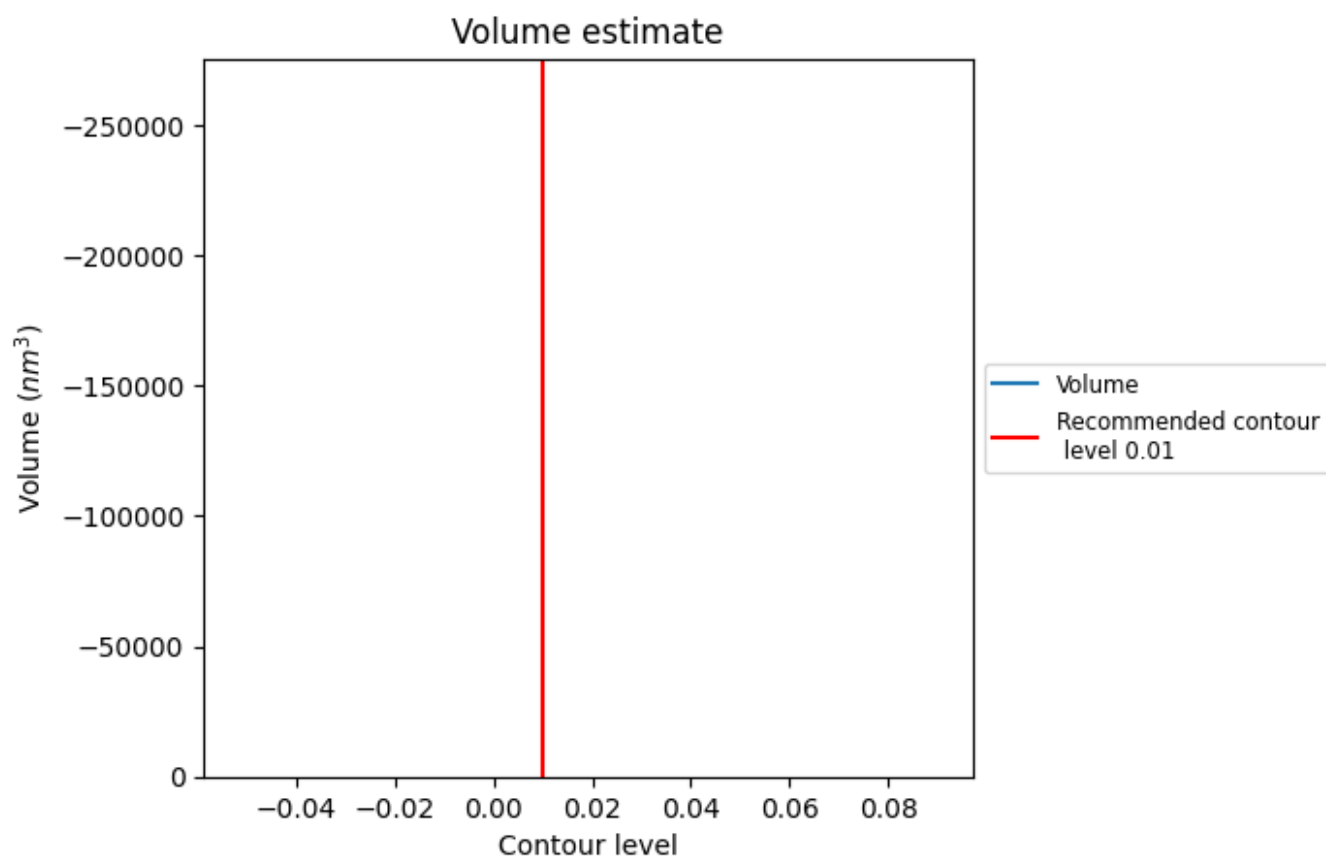
This section contains the results of statistical analysis of the map.

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 -2386571 nm³; this corresponds to an approximate mass of -2155852 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.

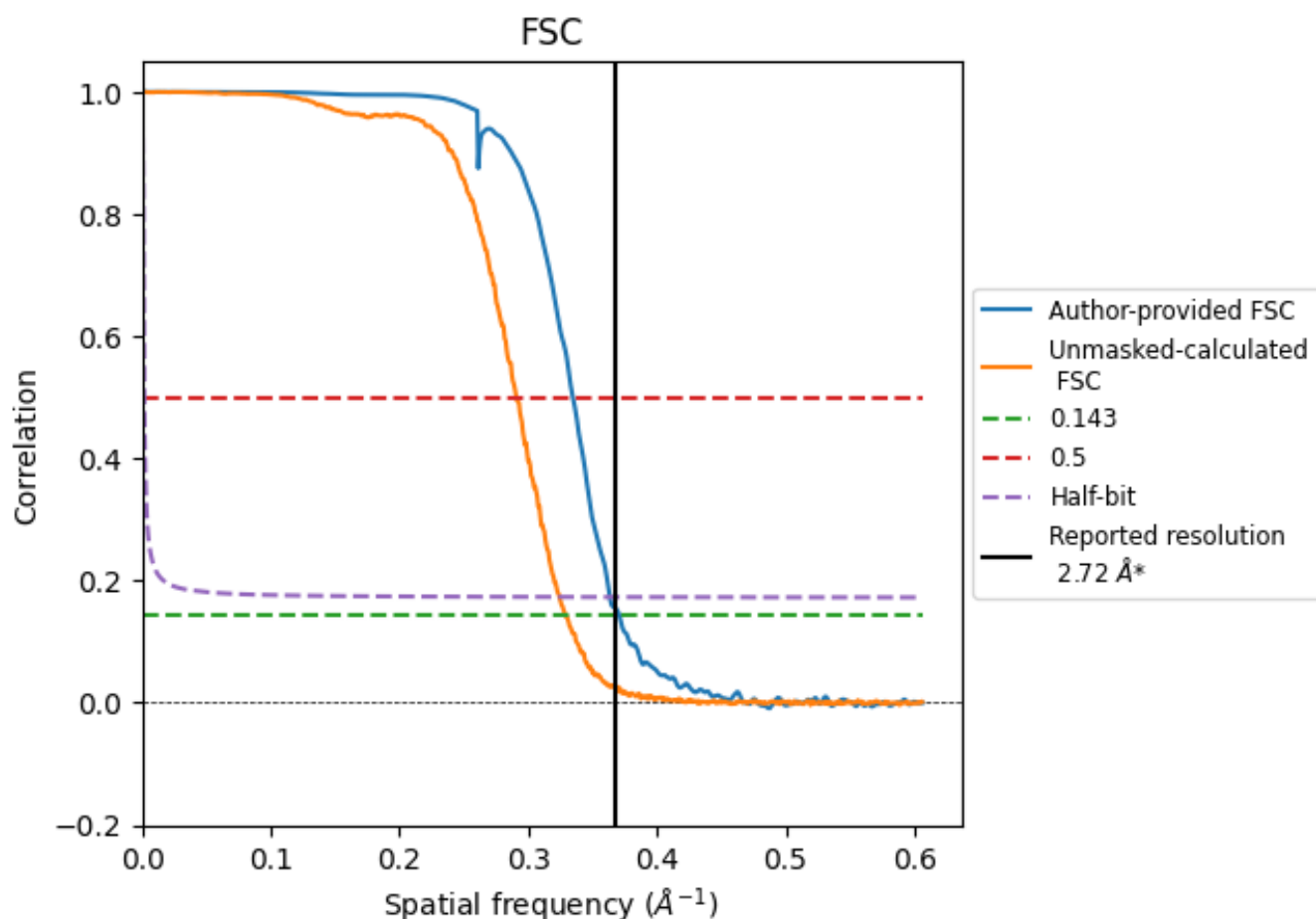
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum could not be displayed.

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 0.368 \AA^{-1}

8.2 Resolution estimates [i](#)

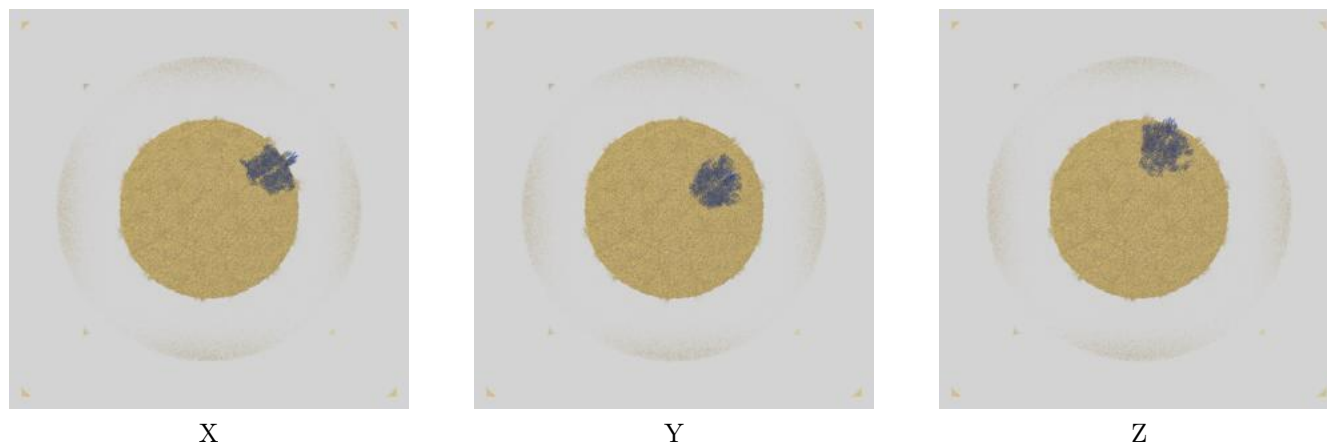
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.70	2.99	2.75
Unmasked-calculated*	3.04	3.44	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.04 differs from the reported value 2.72 by more than 10 %

9 Map-model fit [i](#)

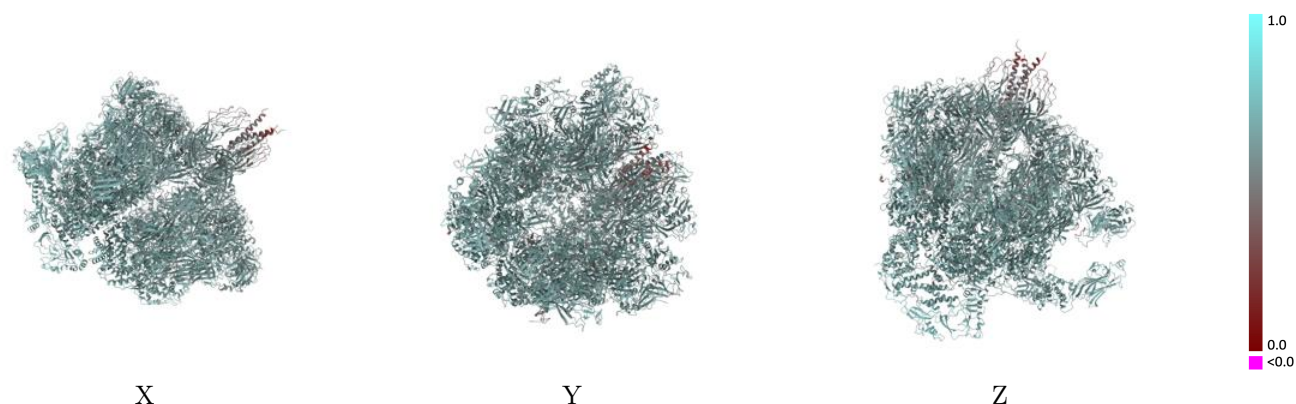
This section contains information regarding the fit between EMDB map EMD-45121 and PDB model 9C1J. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



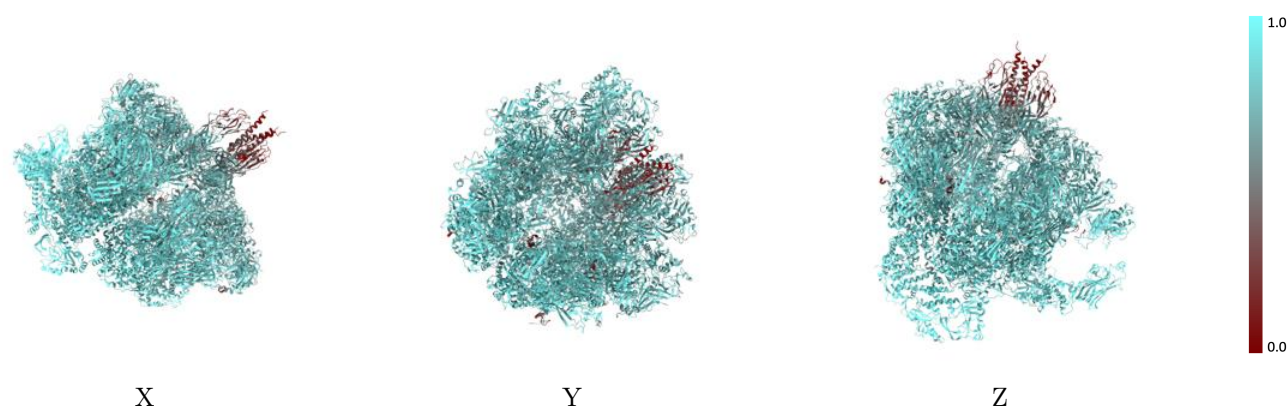
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



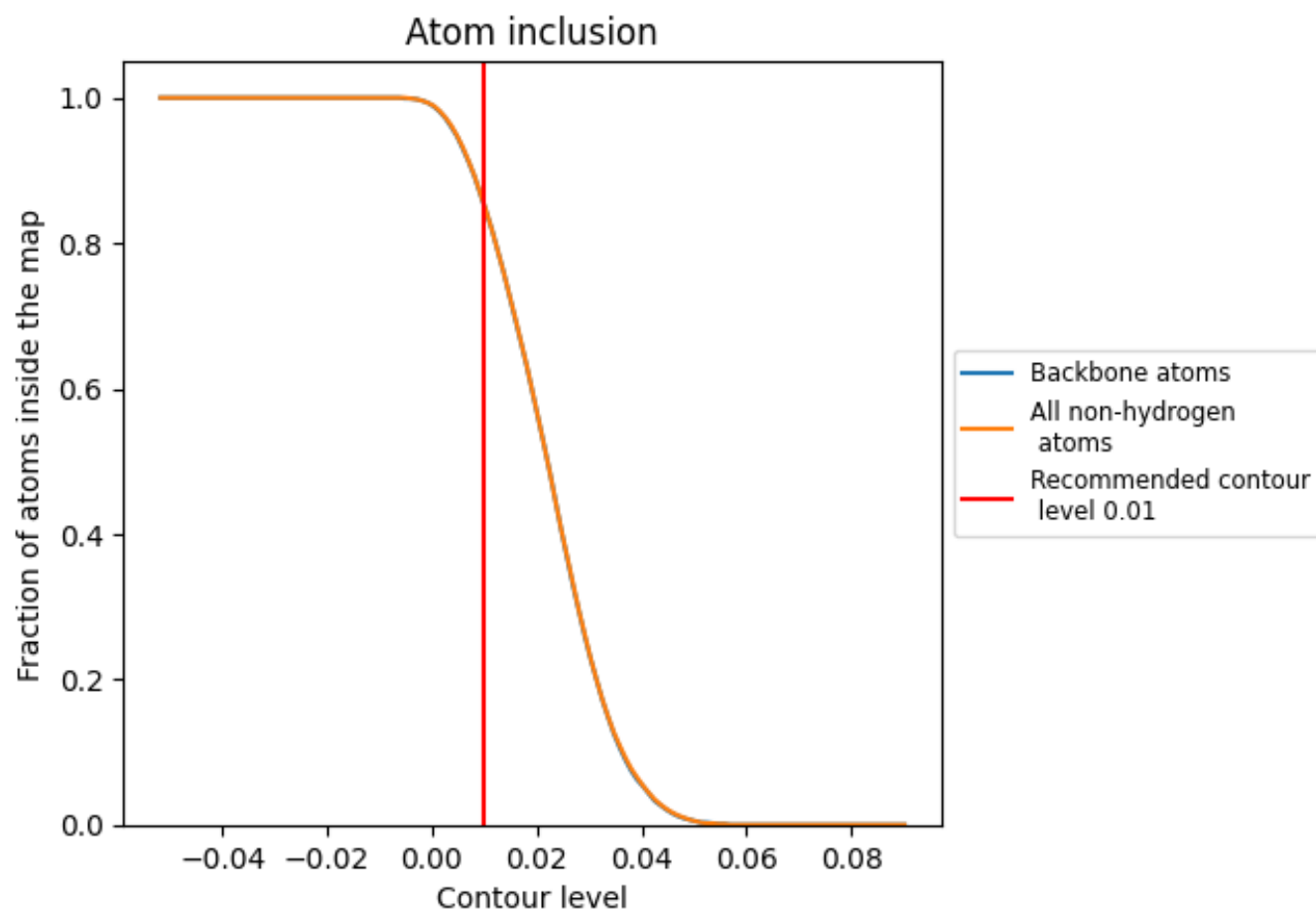
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8520	 0.6110
0	 0.7990	 0.5900
1	 0.8100	 0.5900
2	 0.5220	 0.5220
3	 0.5370	 0.5140
4	 0.5280	 0.5170
A	 0.9370	 0.6390
B	 0.9280	 0.6340
C	 0.9190	 0.6260
D	 0.9260	 0.6320
E	 0.9200	 0.6340
F	 0.9140	 0.6290
G	 0.9190	 0.6290
H	 0.9150	 0.6300
I	 0.9260	 0.6340
J	 0.9270	 0.6300
K	 0.9160	 0.6300
L	 0.9250	 0.6300
M	 0.9230	 0.6310
N	 0.9280	 0.6330
O	 0.9250	 0.6310
P	 0.8170	 0.5910
Q	 0.7870	 0.5880
R	 0.8020	 0.5930
S	 0.8070	 0.5910
T	 0.7930	 0.5860
U	 0.7840	 0.5870
V	 0.7930	 0.5860
W	 0.7870	 0.5880
X	 0.7830	 0.5900
Y	 0.8080	 0.5980
Z	 0.8130	 0.5900
f	 0.9160	 0.6290
g	 0.9120	 0.6250
h	 0.9240	 0.6300



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Chain	Atom inclusion	Q-score
i	 0.9290	 0.6320
j	 0.9270	 0.6310
k	 0.9170	 0.6280
t	 0.8000	 0.5870
u	 0.7860	 0.5890
v	 0.7930	 0.5880
w	 0.7750	 0.5870
x	 0.7710	 0.5840
y	 0.7990	 0.5930