wwPDB EM Validation Summary Report

Jan 20, 2024 – 07:07 am GMT

PDB ID	:	8OPL
EMDB ID	:	EMD-17072
Title	:	Virus-like Particle based on PVY coat protein with T43C and D136C mutation with helical architecture encapsidating ssRNA
Authors	:	Kavcic, L.; Kezar, A.; Podobnik, M.
Deposited on	:	2023-04-07
Resolution	:	2.41 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:

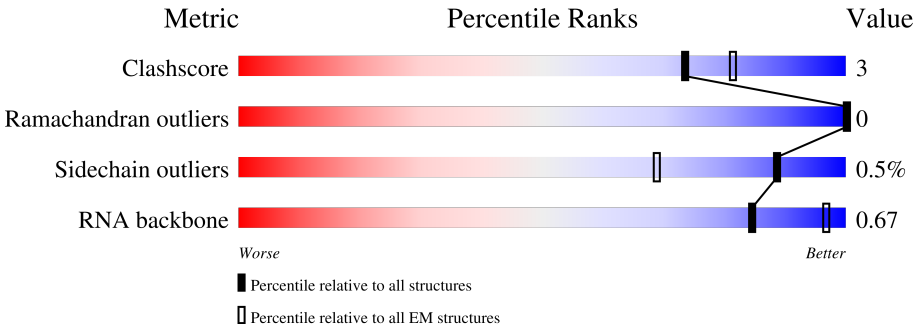
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.41 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	Aa	267	19% 84% 16%
1	Ab	267	19% 84% 16%
1	Ac	267	19% 84% 16%
1	Ad	267	20% 84% 16%
1	Ae	267	19% 84% 16%
1	Af	267	19% 84% 16%
1	Ag	267	20% 84% 16%

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Mol	Chain	Length	Quality of chain
1	Ah	267	19% 84% 16%
1	Ai	267	19% 84% 16%
1	As	267	20% 84% 16%
1	At	267	18% 84% 16%
1	Au	267	19% 84% 16%
1	Av	267	19% 84% 16%
1	Aw	267	19% 84% 16%
1	Ax	267	19% 84% 16%
1	Ay	267	19% 84% 16%
1	Az	267	19% 84% 16%
1	Ba	267	19% 84% 16%
1	Bk	267	19% 84% 16%
1	Bl	267	19% 84% 16%
1	Bm	267	18% 84% 16%
1	Bn	267	19% 84% 16%
1	Bo	267	20% 84% 16%
1	Bp	267	19% 84% 16%
1	Bq	267	18% 84% 16%
1	Br	267	19% 84% 16%
1	Bs	267	18% 84% 16%
2	Aj	5	100%
2	Ak	5	100%
2	Al	5	100%
2	Am	5	100%
2	An	5	100%

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Mol	Chain	Length	Quality of chain
2	Ao	5	100%
2	Ap	5	100%
2	Aq	5	100%
2	Ar	5	100%
2	Bb	5	100%
2	Bc	5	100%
2	Bd	5	100%
2	Be	5	100%
2	Bf	5	100%
2	Bg	5	100%
2	Bh	5	100%
2	Bi	5	100%
2	Bj	5	100%
2	Bt	5	100%
2	Bu	5	100%
2	Bv	5	100%
2	Bw	5	100%
2	Bx	5	100%
2	By	5	100%
2	Bz	5	100%
2	Ca	5	100%
2	Cb	5	100%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 50679 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Genome polyprotein (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ab	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ac	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ad	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ae	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Af	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ag	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ah	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ai	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	As	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	At	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Au	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Av	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Aw	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ax	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Ay	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Az	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ba	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Bk	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Bl	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Bm	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Bn	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Bo	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Bp	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Bq	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Br	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		
1	Bs	224	Total	C	N	O	S	0	0
			1777	1114	311	337	15		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	43	CYS	THR	engineered mutation	UNP I7DGZ0
Aa	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ab	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ab	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ac	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ac	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ad	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ad	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ae	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ae	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Af	43	CYS	THR	engineered mutation	UNP I7DGZ0
Af	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ag	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ag	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ah	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ah	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ai	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ai	136	CYS	ASP	engineered mutation	UNP I7DGZ0
As	43	CYS	THR	engineered mutation	UNP I7DGZ0

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Chain	Residue	Modelled	Actual	Comment	Reference
As	136	CYS	ASP	engineered mutation	UNP I7DGZ0
At	43	CYS	THR	engineered mutation	UNP I7DGZ0
At	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Au	43	CYS	THR	engineered mutation	UNP I7DGZ0
Au	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Av	43	CYS	THR	engineered mutation	UNP I7DGZ0
Av	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Aw	43	CYS	THR	engineered mutation	UNP I7DGZ0
Aw	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ax	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ax	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ay	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ay	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Az	43	CYS	THR	engineered mutation	UNP I7DGZ0
Az	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Ba	43	CYS	THR	engineered mutation	UNP I7DGZ0
Ba	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Bk	43	CYS	THR	engineered mutation	UNP I7DGZ0
Bk	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Bl	43	CYS	THR	engineered mutation	UNP I7DGZ0
Bl	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Bm	43	CYS	THR	engineered mutation	UNP I7DGZ0
Bm	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Bn	43	CYS	THR	engineered mutation	UNP I7DGZ0
Bn	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Bo	43	CYS	THR	engineered mutation	UNP I7DGZ0
Bo	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Bp	43	CYS	THR	engineered mutation	UNP I7DGZ0
Bp	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Bq	43	CYS	THR	engineered mutation	UNP I7DGZ0
Bq	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Br	43	CYS	THR	engineered mutation	UNP I7DGZ0
Br	136	CYS	ASP	engineered mutation	UNP I7DGZ0
Bs	43	CYS	THR	engineered mutation	UNP I7DGZ0
Bs	136	CYS	ASP	engineered mutation	UNP I7DGZ0

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Aj	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Ak	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Al	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Am	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	An	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Ao	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Ap	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Aq	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Ar	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bb	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bc	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bd	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Be	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bf	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bg	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bh	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bi	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bj	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bt	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bu	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bv	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bw	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bx	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

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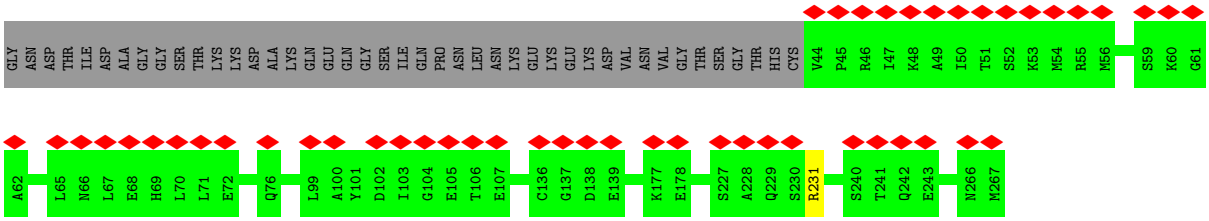
Mol	Chain	Residues	Atoms					AltConf	Trace
2	By	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Bz	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Ca	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Cb	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

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.

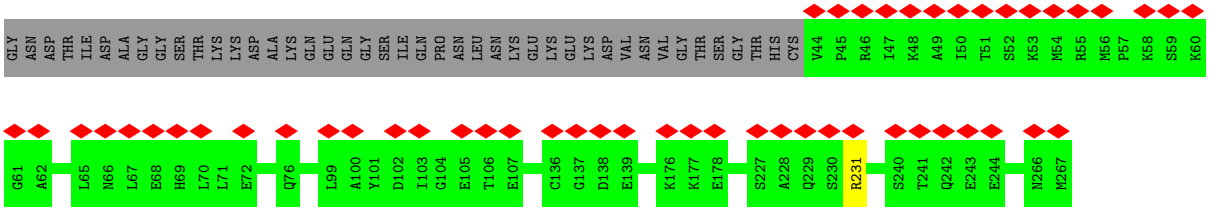
• Molecule 1: Genome polyprotein (Fragment)

Chain Aa:



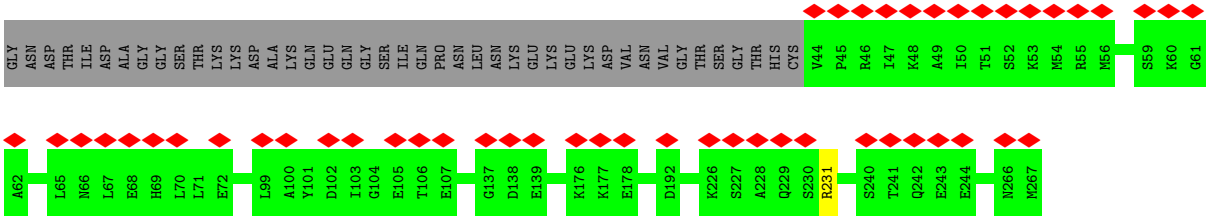
• Molecule 1: Genome polyprotein (Fragment)

Chain Ab:



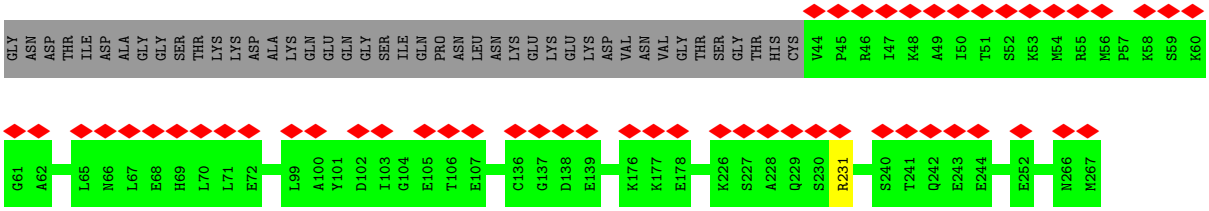
• Molecule 1: Genome polyprotein (Fragment)

Chain Ac:

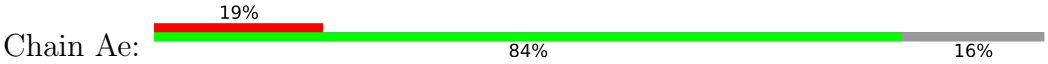


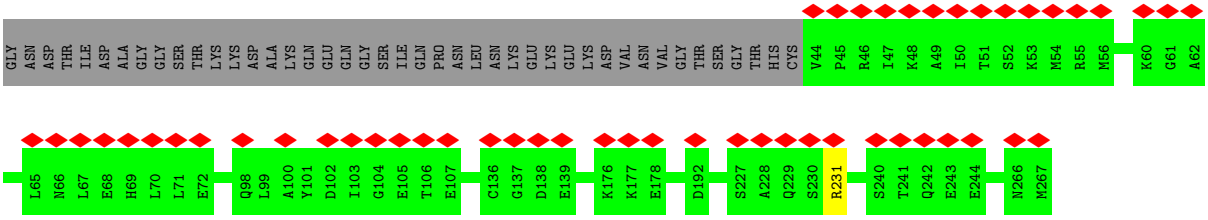
• Molecule 1: Genome polyprotein (Fragment)

Chain Ad:

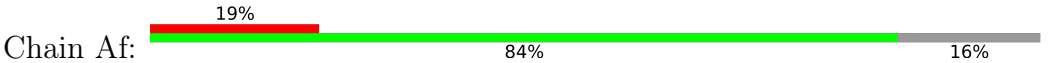


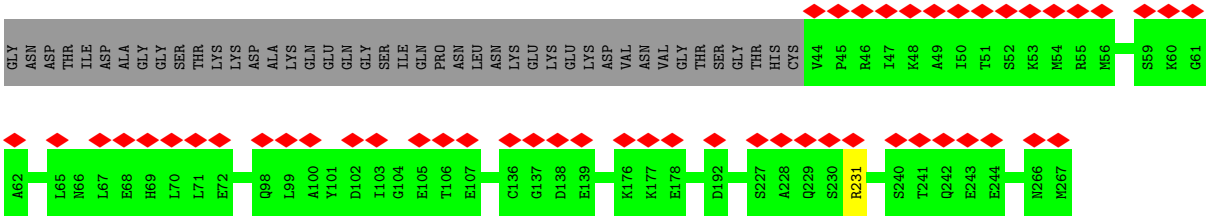
• Molecule 1: Genome polyprotein (Fragment)



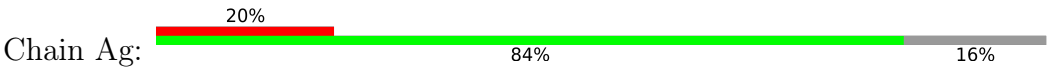


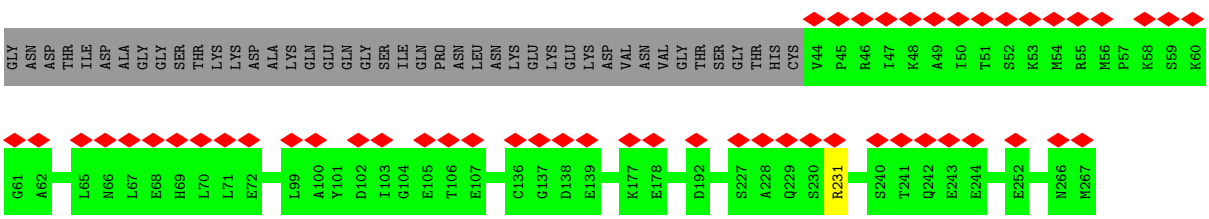
• Molecule 1: Genome polyprotein (Fragment)



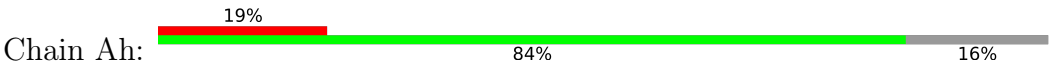


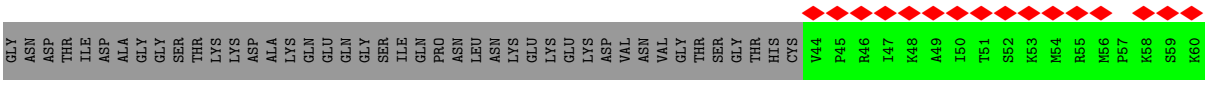
• Molecule 1: Genome polyprotein (Fragment)

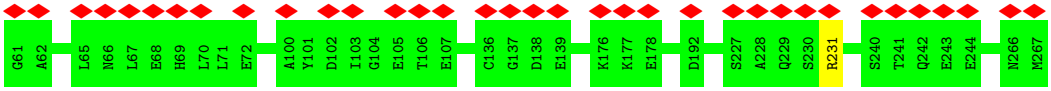




• Molecule 1: Genome polyprotein (Fragment)

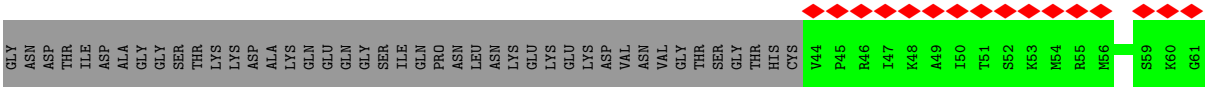


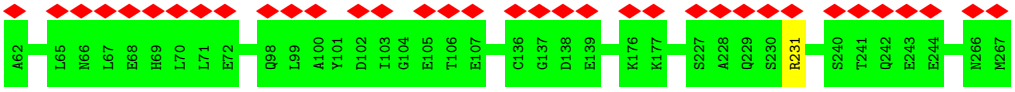




• Molecule 1: Genome polyprotein (Fragment)

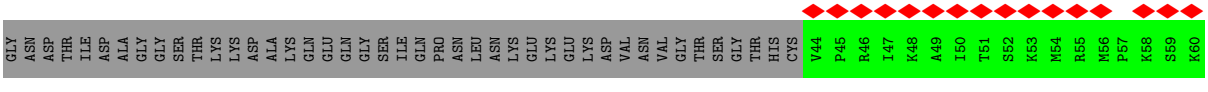
Chain Ai:

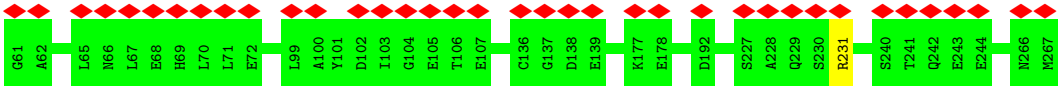




• Molecule 1: Genome polyprotein (Fragment)

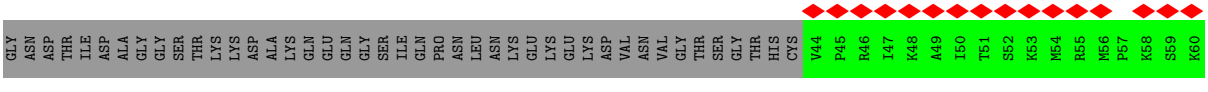
Chain As:

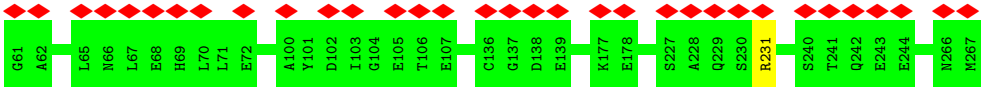




• Molecule 1: Genome polyprotein (Fragment)

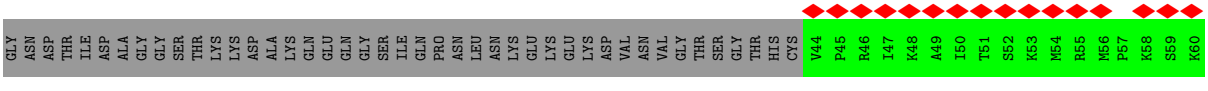
Chain At:

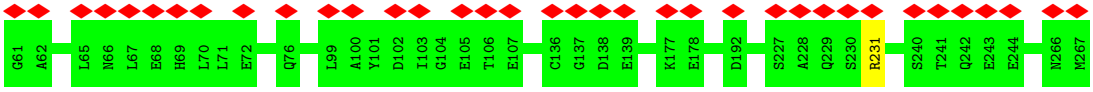




• Molecule 1: Genome polyprotein (Fragment)

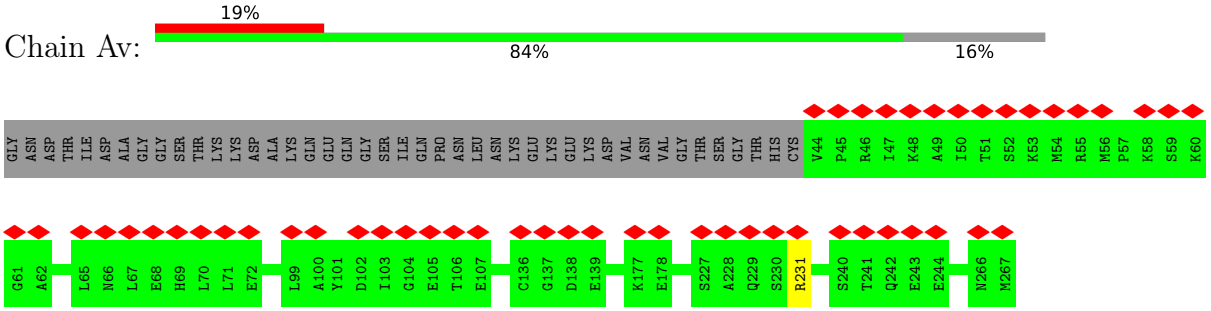
Chain Au:





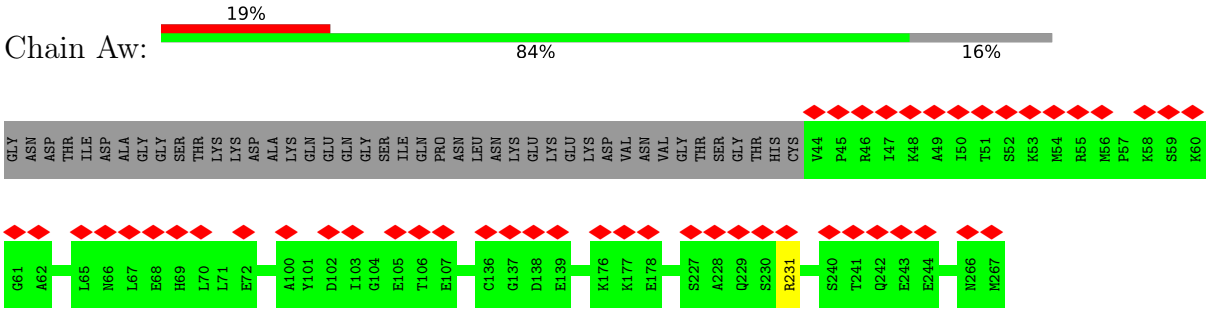
• Molecule 1: Genome polyprotein (Fragment)

Chain Av:



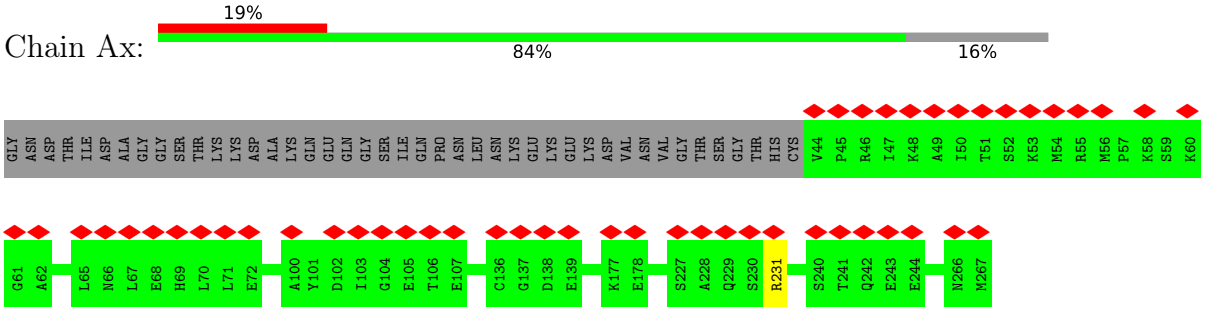
• Molecule 1: Genome polyprotein (Fragment)

Chain Aw:



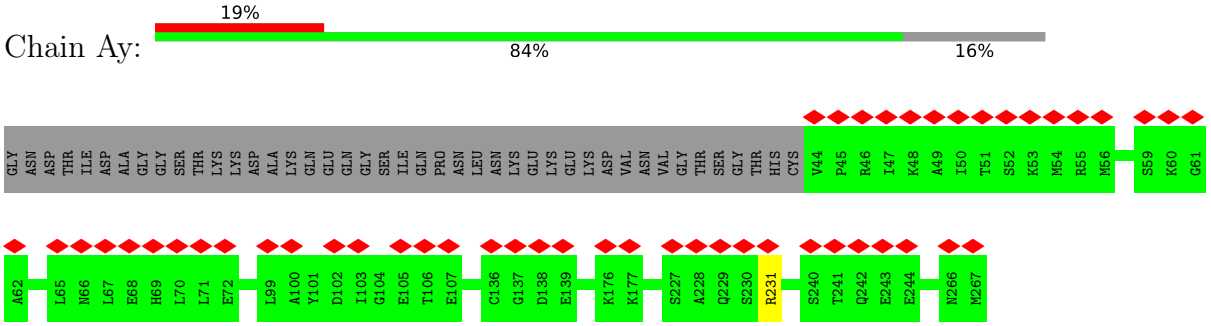
• Molecule 1: Genome polyprotein (Fragment)

Chain Ax:



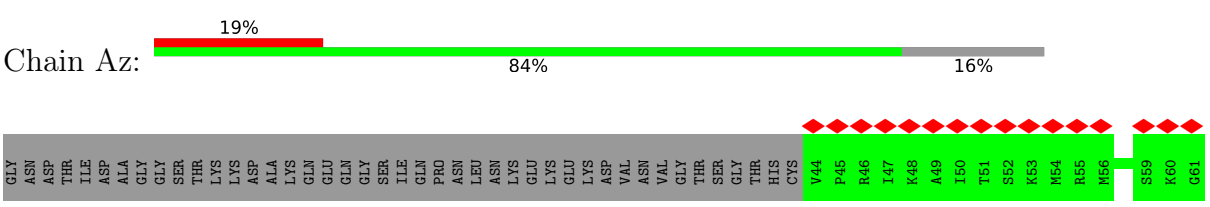
• Molecule 1: Genome polyprotein (Fragment)

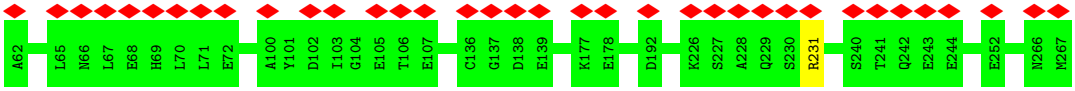
Chain Ay:



• Molecule 1: Genome polyprotein (Fragment)

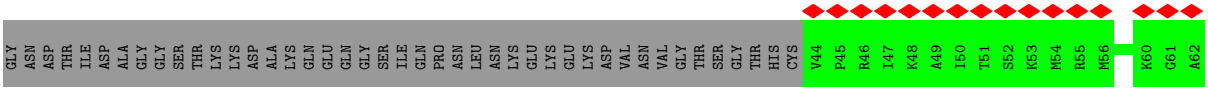
Chain Az:

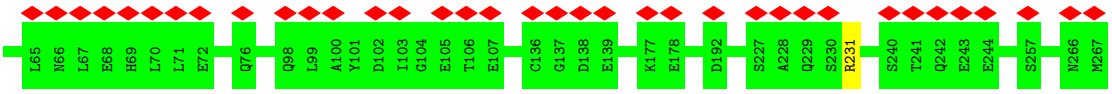




• Molecule 1: Genome polyprotein (Fragment)

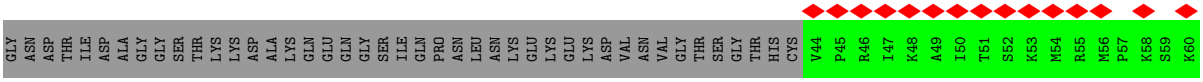
Chain Ba:

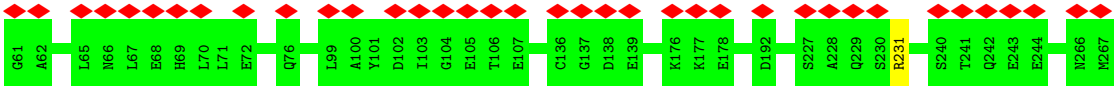




• Molecule 1: Genome polyprotein (Fragment)

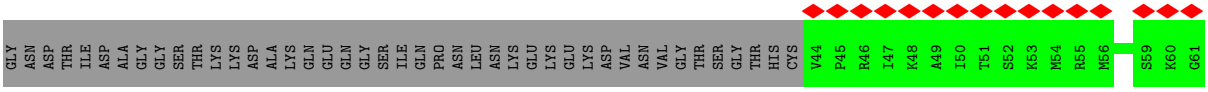
Chain Bk:

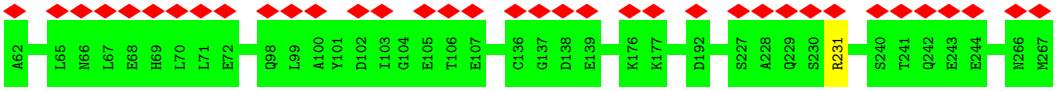




• Molecule 1: Genome polyprotein (Fragment)

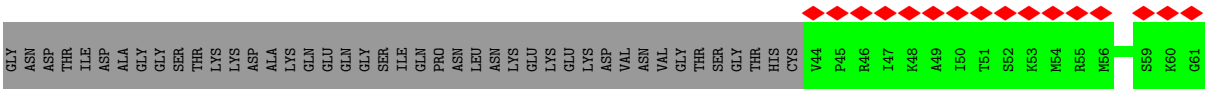
Chain Bl:

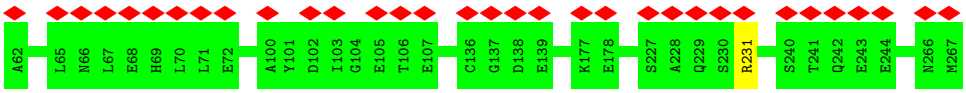




• Molecule 1: Genome polyprotein (Fragment)

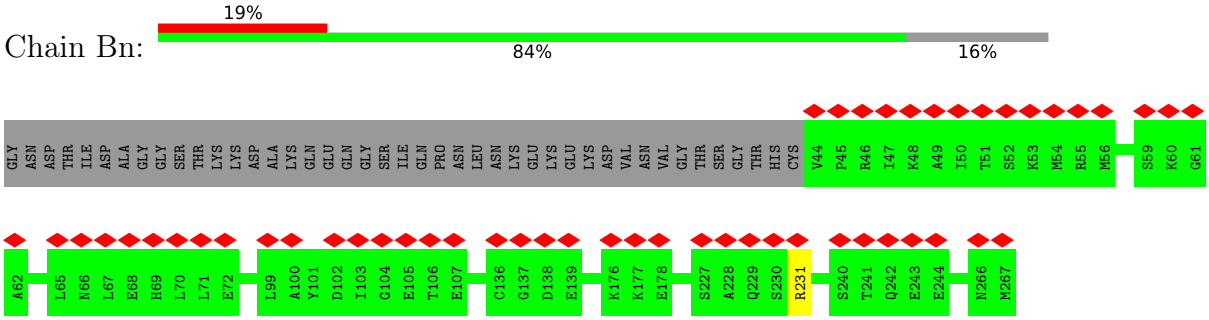
Chain Bm:





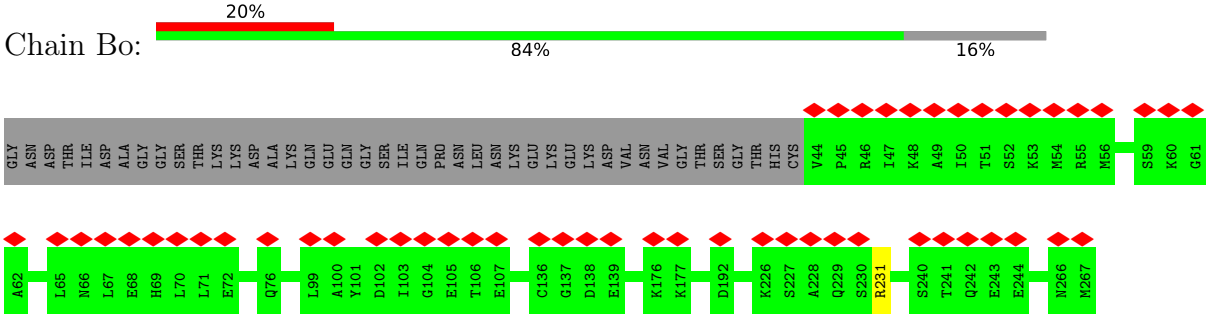
• Molecule 1: Genome polyprotein (Fragment)

Chain Bn:



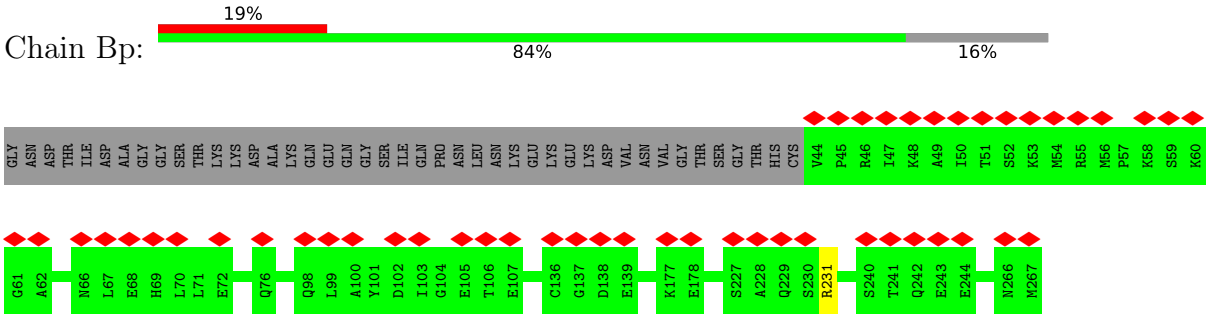
• Molecule 1: Genome polyprotein (Fragment)

Chain Bo:



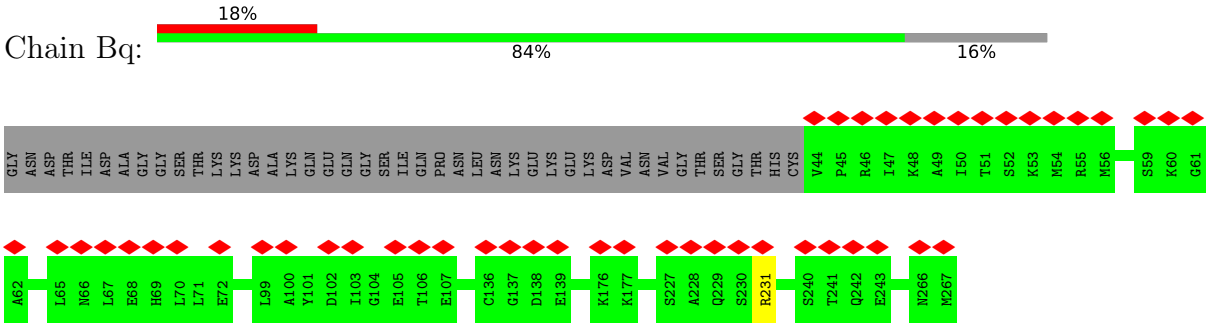
• Molecule 1: Genome polyprotein (Fragment)

Chain Bp:



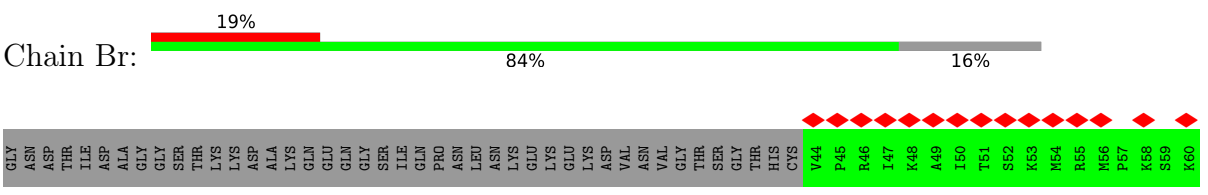
• Molecule 1: Genome polyprotein (Fragment)

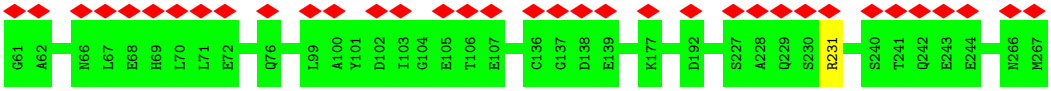
Chain Bq:



• Molecule 1: Genome polyprotein (Fragment)

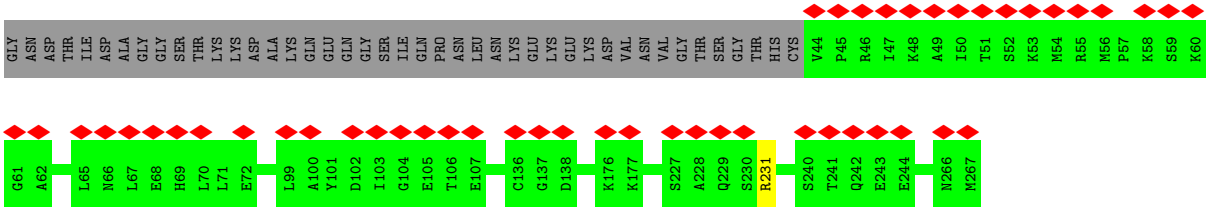
Chain Br:





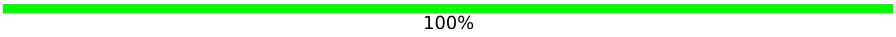
• Molecule 1: Genome polyprotein (Fragment)

Chain Bs:



• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

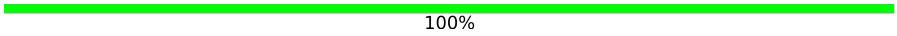
Chain Aj:



There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ak:



There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Al:

There are no outlier residues recorded for this chain.

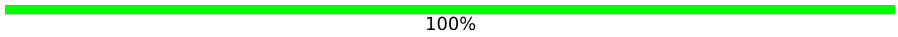
• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Am:

There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

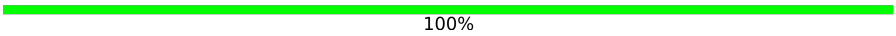
Chain An:



There are no outlier residues recorded for this chain.

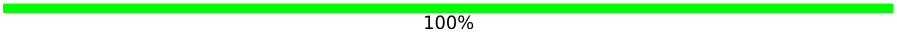
• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ao:



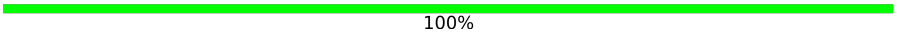
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ap: 

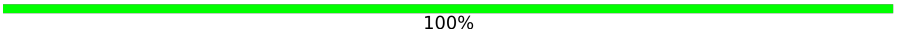
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Aq: 

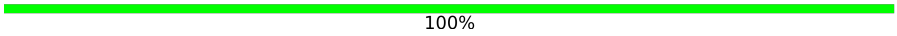
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ar: 

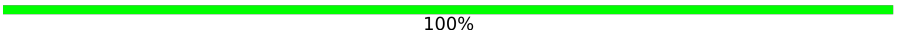
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bb: 

There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bc: 

There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bd: 

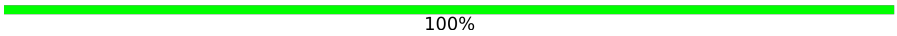
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Be: 

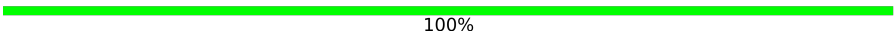
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bf: 

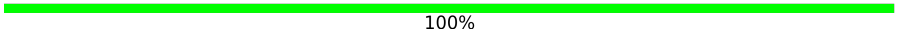
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bg: 

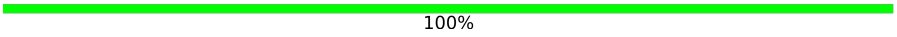
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bh: 

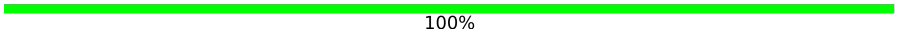
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bi: 

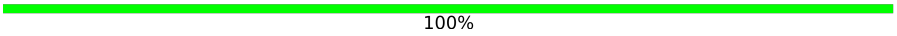
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bj: 

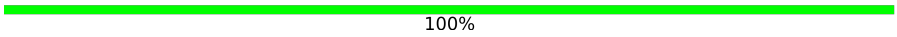
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bt: 

There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bu: 

There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bv: 

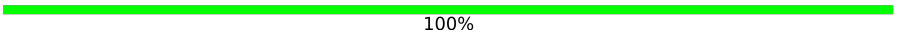
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bw: 

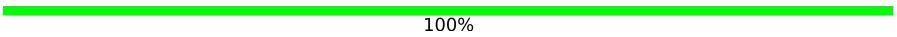
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bx: 

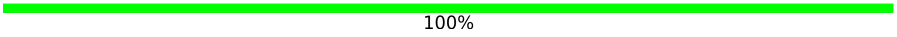
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain By: 

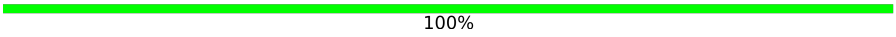
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bz: 

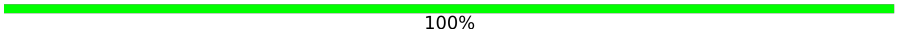
There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ca: 

There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cb: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-40.997°, rise=4.005 Å, axial sym=C1	Depositor
Number of segments used	141112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND-4.1	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	11.224	Depositor
Minimum map value	-5.395	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.551	Depositor
Recommended contour level	2.22	Depositor
Map size (Å)	285.0, 285.0, 285.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	Aa	0.28	0/1813	0.49	0/2454
1	Ab	0.28	0/1813	0.49	0/2454
1	Ac	0.28	0/1813	0.49	0/2454
1	Ad	0.28	0/1813	0.50	0/2454
1	Ae	0.28	0/1813	0.49	0/2454
1	Af	0.28	0/1813	0.49	0/2454
1	Ag	0.28	0/1813	0.49	0/2454
1	Ah	0.28	0/1813	0.49	0/2454
1	Ai	0.28	0/1813	0.49	0/2454
1	As	0.28	0/1813	0.50	0/2454
1	At	0.28	0/1813	0.49	0/2454
1	Au	0.28	0/1813	0.49	0/2454
1	Av	0.28	0/1813	0.50	0/2454
1	Aw	0.28	0/1813	0.49	0/2454
1	Ax	0.28	0/1813	0.49	0/2454
1	Ay	0.28	0/1813	0.49	0/2454
1	Az	0.28	0/1813	0.49	0/2454
1	Ba	0.28	0/1813	0.49	0/2454
1	Bk	0.28	0/1813	0.49	0/2454
1	Bl	0.28	0/1813	0.49	0/2454
1	Bm	0.28	0/1813	0.49	0/2454
1	Bn	0.28	0/1813	0.49	0/2454
1	Bo	0.28	0/1813	0.49	0/2454
1	Bp	0.28	0/1813	0.49	0/2454
1	Bq	0.28	0/1813	0.49	0/2454
1	Br	0.28	0/1813	0.49	0/2454
1	Bs	0.28	0/1813	0.49	0/2454
2	Aj	0.25	0/109	0.89	0/166
2	Ak	0.26	0/109	0.88	0/166
2	Al	0.25	0/109	0.88	0/166
2	Am	0.25	0/109	0.89	0/166
2	An	0.26	0/109	0.88	0/166
2	Ao	0.26	0/109	0.88	0/166
2	Ap	0.27	0/109	0.88	0/166

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	Aq	0.26	0/109	0.88	0/166
2	Ar	0.26	0/109	0.88	0/166
2	Bb	0.26	0/109	0.88	0/166
2	Bc	0.25	0/109	0.89	0/166
2	Bd	0.26	0/109	0.88	0/166
2	Be	0.26	0/109	0.88	0/166
2	Bf	0.26	0/109	0.88	0/166
2	Bg	0.25	0/109	0.89	0/166
2	Bh	0.25	0/109	0.89	0/166
2	Bi	0.25	0/109	0.88	0/166
2	Bj	0.25	0/109	0.88	0/166
2	Bt	0.27	0/109	0.88	0/166
2	Bu	0.25	0/109	0.88	0/166
2	Bv	0.26	0/109	0.88	0/166
2	Bw	0.25	0/109	0.89	0/166
2	Bx	0.25	0/109	0.88	0/166
2	By	0.25	0/109	0.89	0/166
2	Bz	0.25	0/109	0.89	0/166
2	Ca	0.25	0/109	0.88	0/166
2	Cb	0.26	0/109	0.88	0/166
All	All	0.28	0/51894	0.53	0/70740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	1777	0	1762	0	0
1	Ab	1777	0	1762	0	0
1	Ac	1777	0	1762	0	0
1	Ad	1777	0	1762	0	0
1	Ae	1777	0	1762	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Af	1777	0	1762	0	0
1	Ag	1777	0	1762	0	0
1	Ah	1777	0	1762	0	0
1	Ai	1777	0	1762	0	0
1	As	1777	0	1762	0	0
1	At	1777	0	1762	0	0
1	Au	1777	0	1762	0	0
1	Av	1777	0	1762	0	0
1	Aw	1777	0	1762	0	0
1	Ax	1777	0	1762	0	0
1	Ay	1777	0	1762	0	0
1	Az	1777	0	1762	0	0
1	Ba	1777	0	1762	0	0
1	Bk	1777	0	1762	0	0
1	Bl	1777	0	1762	0	0
1	Bm	1777	0	1762	0	0
1	Bn	1777	0	1762	0	0
1	Bo	1777	0	1762	0	0
1	Bp	1777	0	1762	0	0
1	Bq	1777	0	1762	0	0
1	Br	1777	0	1762	0	0
1	Bs	1777	0	1762	0	0
2	Aj	100	0	51	0	0
2	Ak	100	0	51	0	0
2	Al	100	0	51	0	0
2	Am	100	0	51	0	0
2	An	100	0	51	0	0
2	Ao	100	0	51	0	0
2	Ap	100	0	51	0	0
2	Aq	100	0	51	0	0
2	Ar	100	0	51	0	0
2	Bb	100	0	51	0	0
2	Bc	100	0	51	0	0
2	Bd	100	0	51	0	0
2	Be	100	0	51	0	0
2	Bf	100	0	51	0	0
2	Bg	100	0	51	0	0
2	Bh	100	0	51	0	0
2	Bi	100	0	51	0	0
2	Bj	100	0	51	0	0
2	Bt	100	0	51	0	0
2	Bu	100	0	51	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bv	100	0	51	0	0
2	Bw	100	0	51	0	0
2	Bx	100	0	51	0	0
2	By	100	0	51	0	0
2	Bz	100	0	51	0	0
2	Ca	100	0	51	0	0
2	Cb	100	0	51	0	0
All	All	50679	0	48951	0	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.

There are no clashes within the asymmetric unit.

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	Aa	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ab	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ac	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ad	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ae	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Af	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ag	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ah	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ai	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	As	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	At	222/267 (83%)	221 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Au	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Av	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Aw	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ax	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ay	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Az	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Ba	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Bk	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Bl	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Bm	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Bn	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Bo	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Bp	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Bq	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Br	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
1	Bs	222/267 (83%)	221 (100%)	1 (0%)	0	100	100
All	All	5994/7209 (83%)	5967 (100%)	27 (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	Aa	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ab	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ac	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ad	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ae	194/229 (85%)	193 (100%)	1 (0%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Af	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ag	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ah	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ai	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	As	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	At	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Au	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Av	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Aw	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ax	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ay	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Az	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Ba	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Bk	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Bl	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Bm	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Bn	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Bo	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Bp	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Bq	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Br	194/229 (85%)	193 (100%)	1 (0%)	88	95
1	Bs	194/229 (85%)	193 (100%)	1 (0%)	88	95
All	All	5238/6183 (85%)	5211 (100%)	27 (0%)	89	95

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ax	231	ARG
1	Ba	231	ARG
1	Bq	231	ARG
1	Az	231	ARG
1	Bk	231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Aj	4/5 (80%)	0	0
2	Ak	4/5 (80%)	0	0
2	Al	4/5 (80%)	0	0
2	Am	4/5 (80%)	0	0
2	An	4/5 (80%)	0	0
2	Ao	4/5 (80%)	0	0
2	Ap	4/5 (80%)	0	0
2	Aq	4/5 (80%)	0	0
2	Ar	4/5 (80%)	0	0
2	Bb	4/5 (80%)	0	0
2	Bc	4/5 (80%)	0	0
2	Bd	4/5 (80%)	0	0
2	Be	4/5 (80%)	0	0
2	Bf	4/5 (80%)	0	0
2	Bg	4/5 (80%)	0	0
2	Bh	4/5 (80%)	0	0
2	Bi	4/5 (80%)	0	0
2	Bj	4/5 (80%)	0	0
2	Bt	4/5 (80%)	0	0
2	Bu	4/5 (80%)	0	0
2	Bv	4/5 (80%)	0	0
2	Bw	4/5 (80%)	0	0
2	Bx	4/5 (80%)	0	0
2	By	4/5 (80%)	0	0
2	Bz	4/5 (80%)	0	0
2	Ca	4/5 (80%)	0	0
2	Cb	4/5 (80%)	0	0
All	All	108/135 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

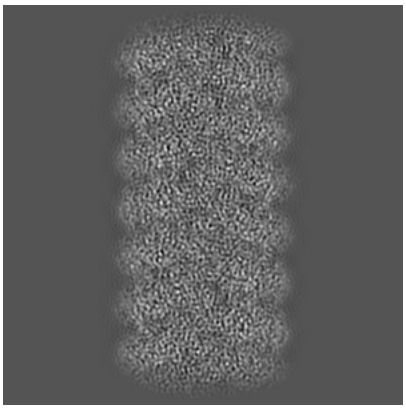
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17072. These allow visual inspection of the internal detail of the map and identification of artifacts.

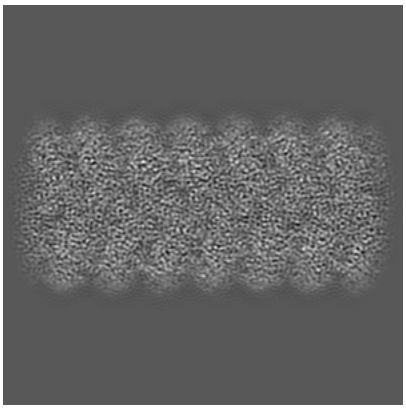
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

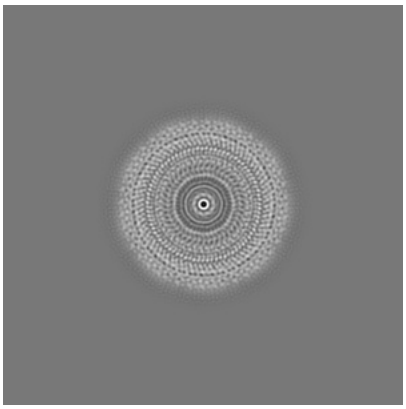
6.1.1 Primary map



X

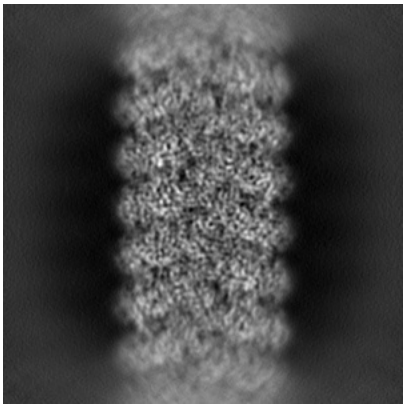


Y

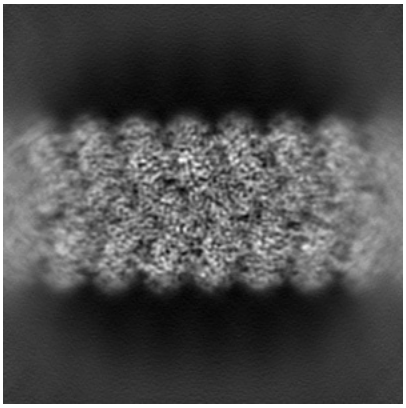


Z

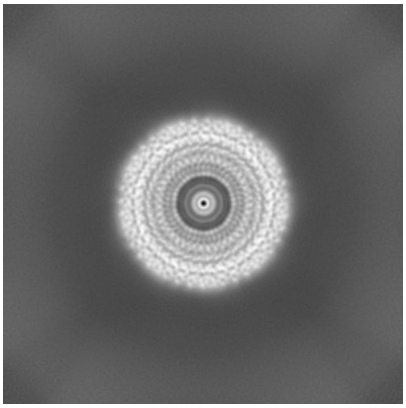
6.1.2 Raw map



X



Y

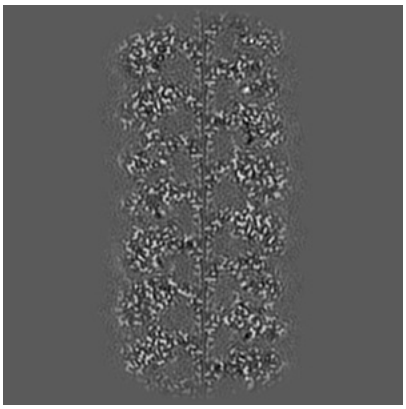


Z

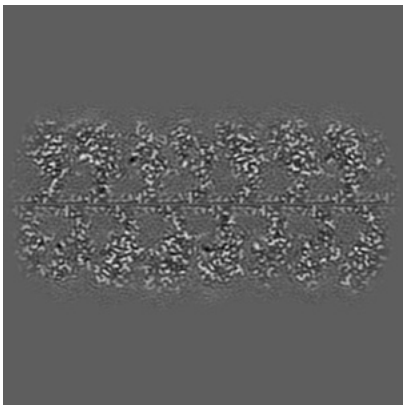
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

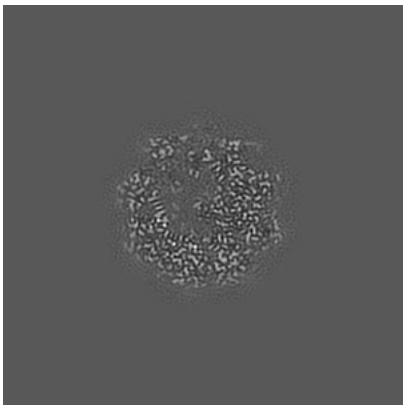
6.2.1 Primary map



X Index: 150

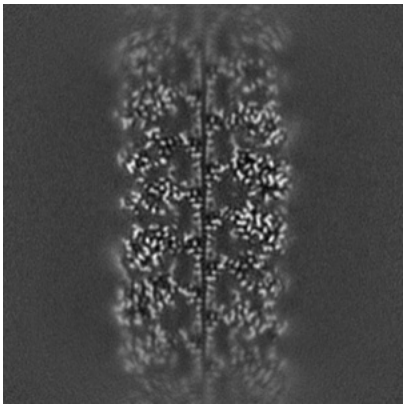


Y Index: 150

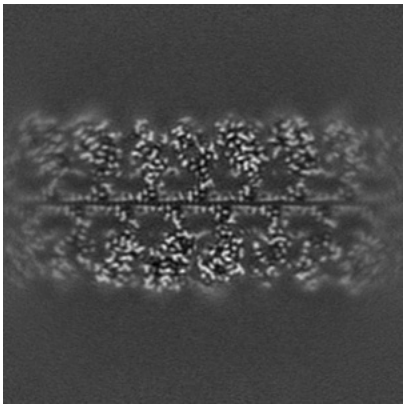


Z Index: 150

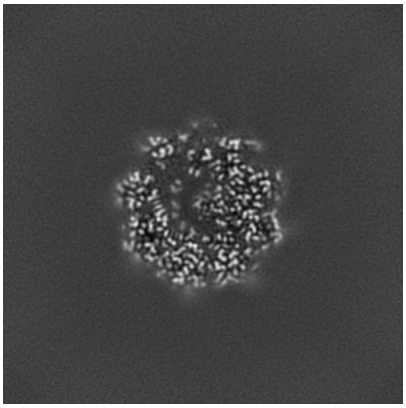
6.2.2 Raw map



X Index: 150



Y Index: 150

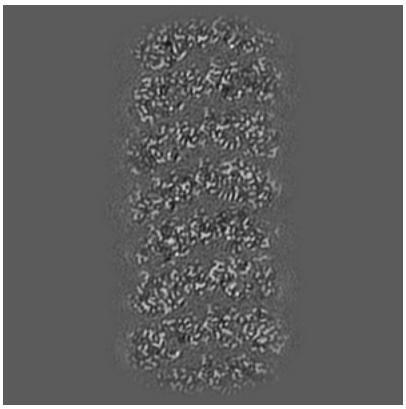


Z Index: 150

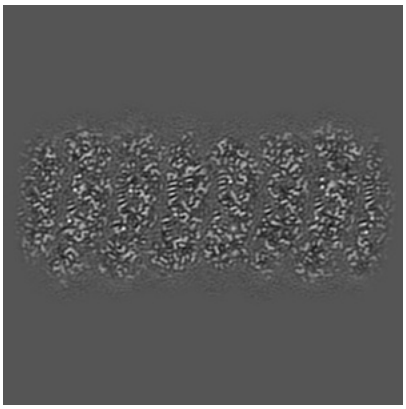
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

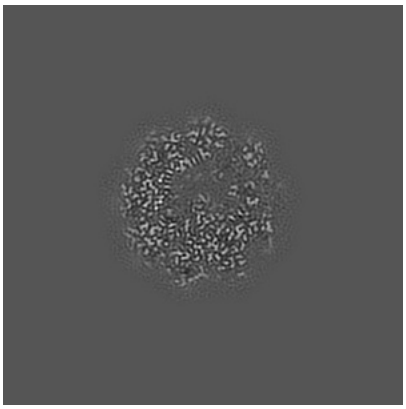
6.3.1 Primary map



X Index: 124

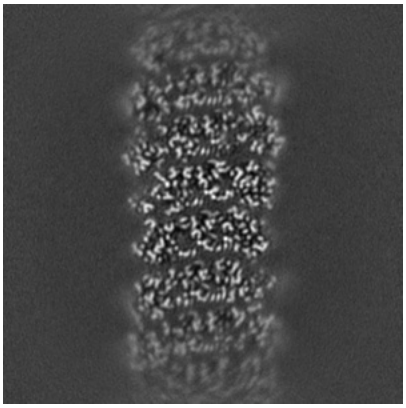


Y Index: 181

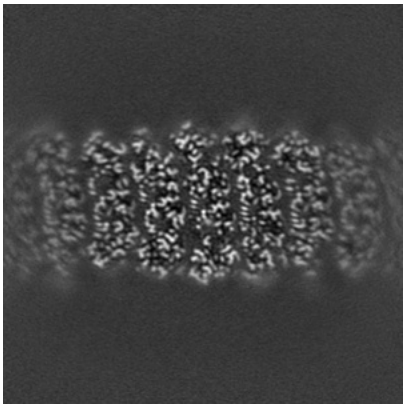


Z Index: 158

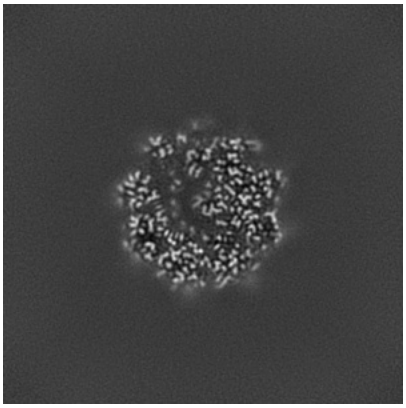
6.3.2 Raw map



X Index: 118



Y Index: 118

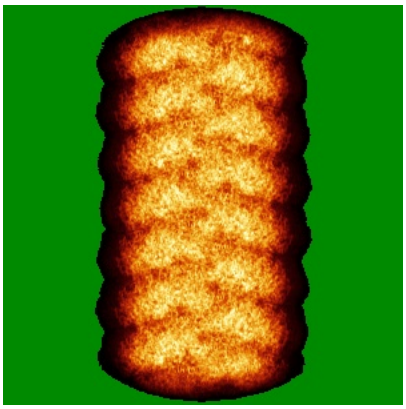


Z Index: 149

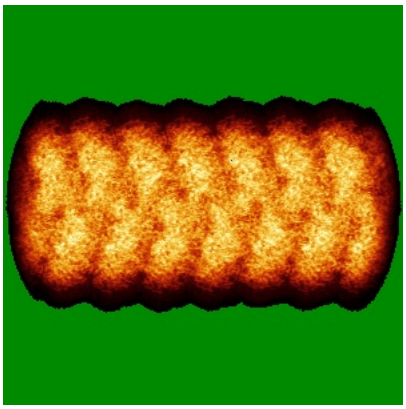
The images above show the largest variance slices of the map in three orthogonal directions.

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

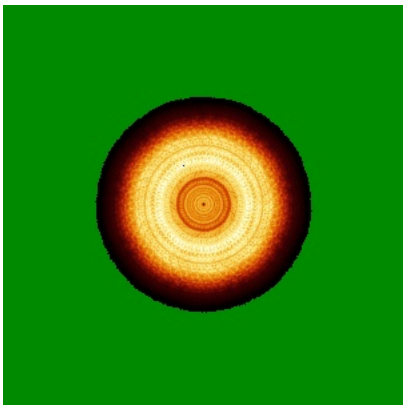
6.4.1 Primary map



X

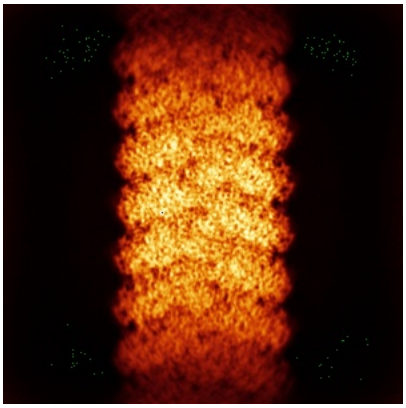


Y

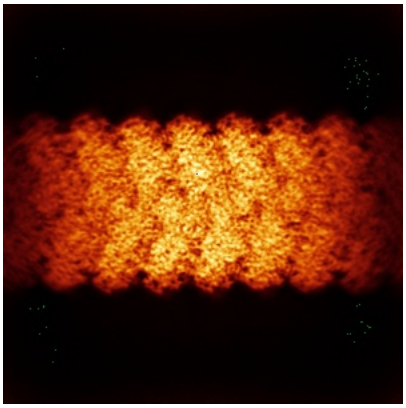


Z

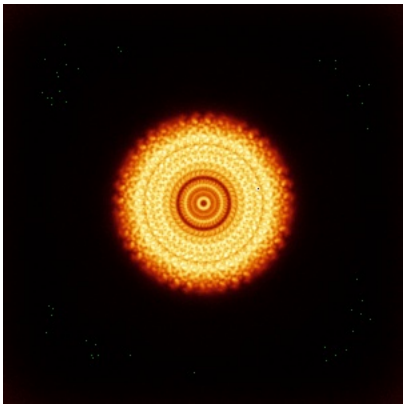
6.4.2 Raw map



X



Y

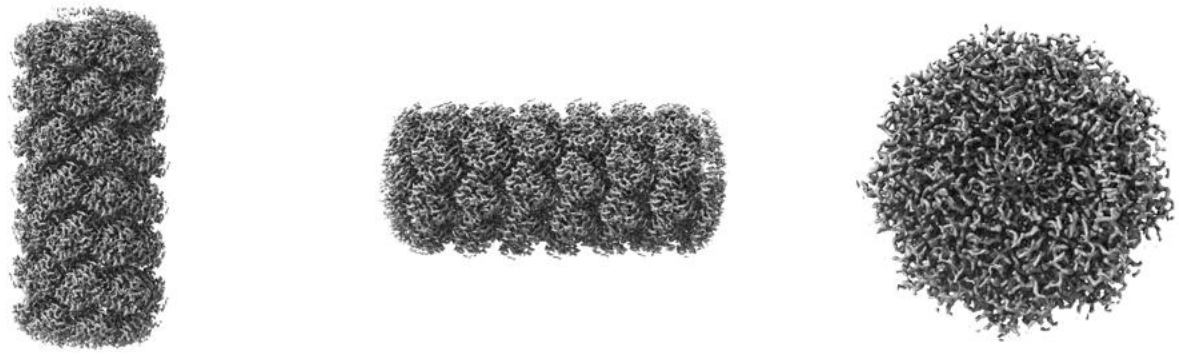


Z

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)

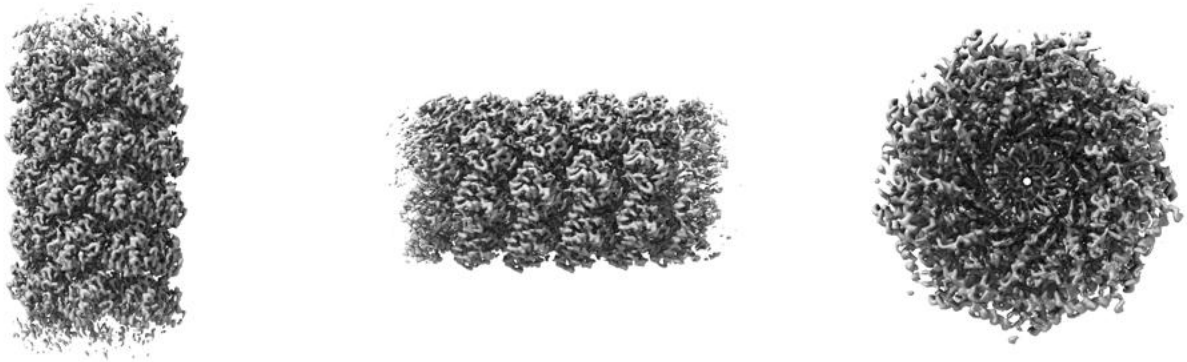
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.22. 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.

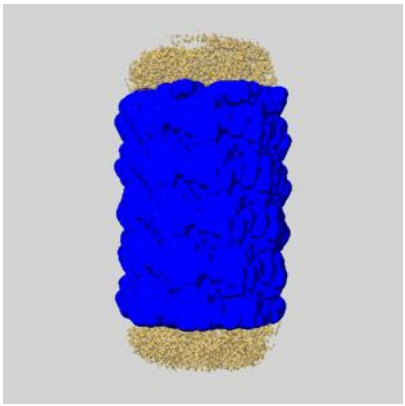
6.6 Mask visualisation (i)

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

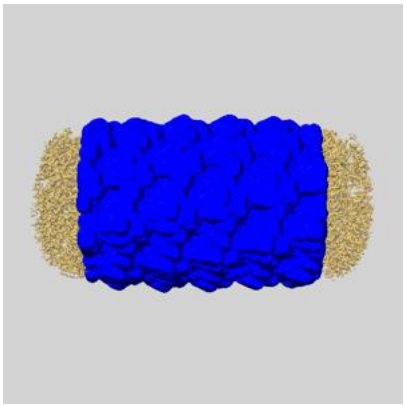
A mask typically either:

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

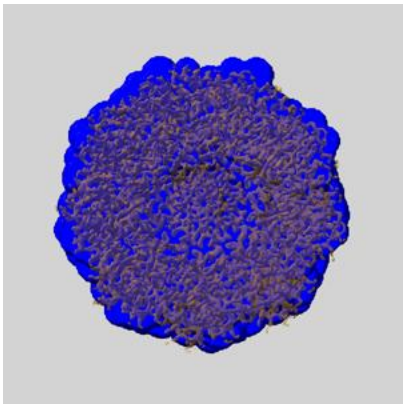
6.6.1 emd_17072_msk_1.map (i)



X



Y

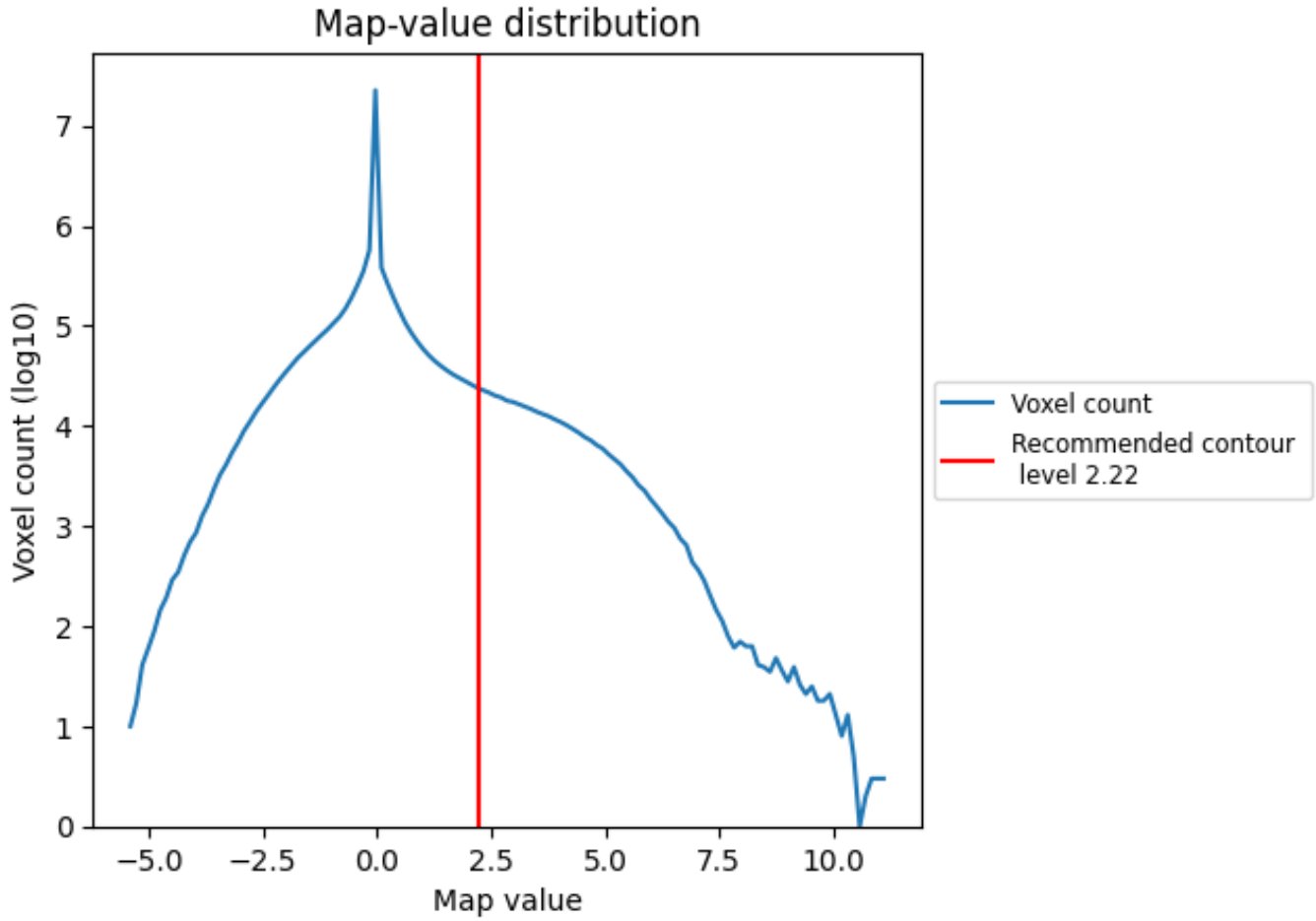


Z

7 Map analysis

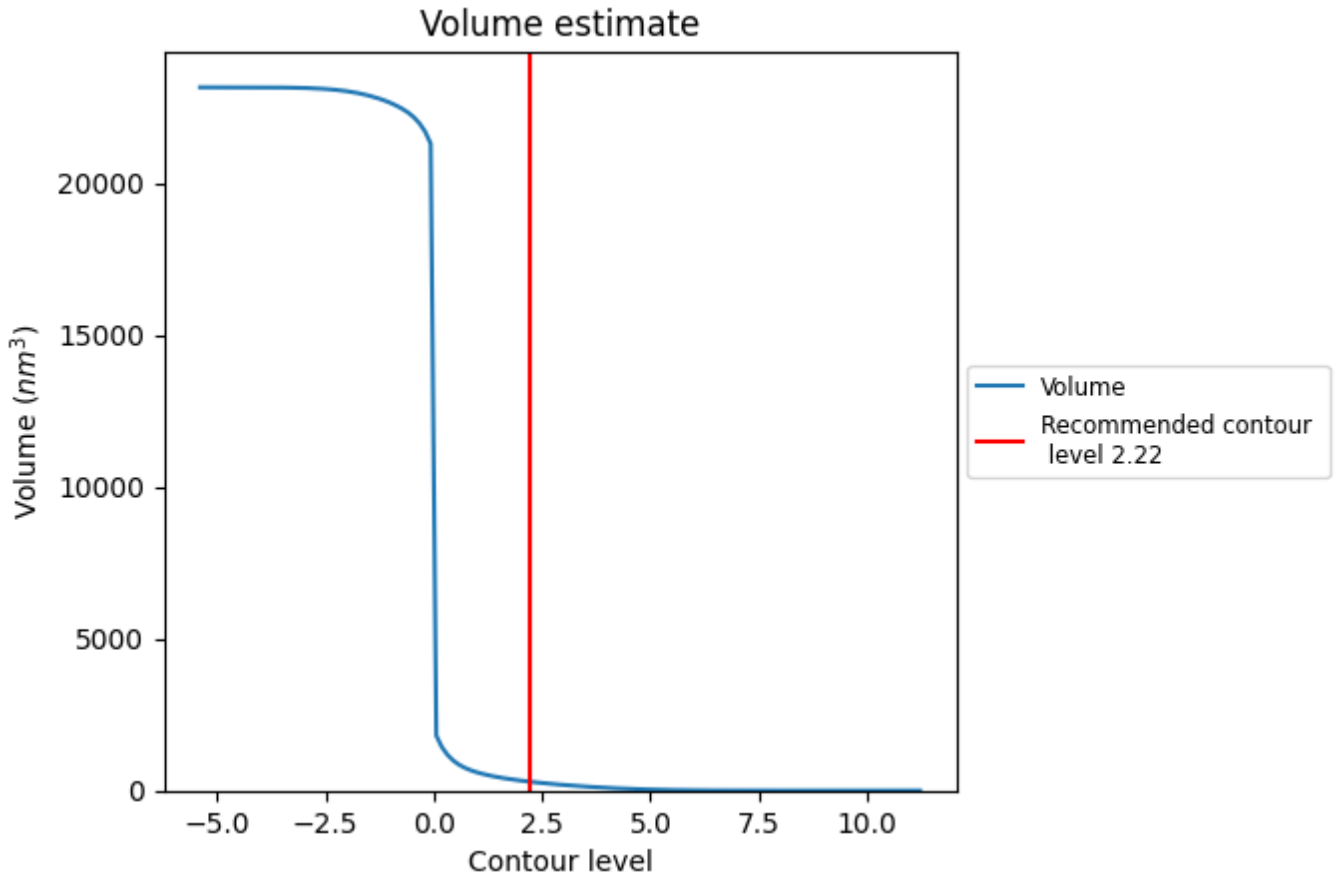
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

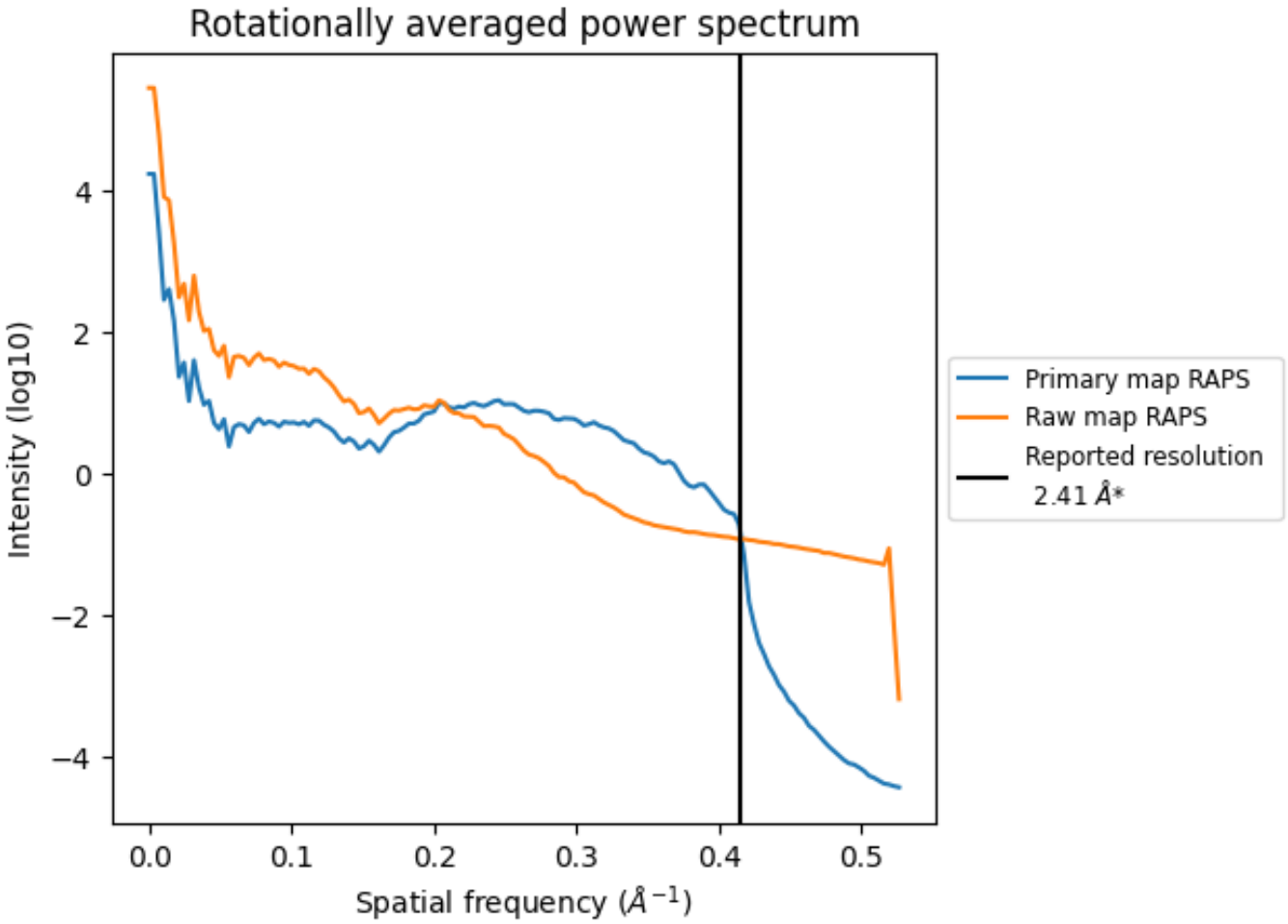
7.2 Volume estimate (i)



The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 263 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)

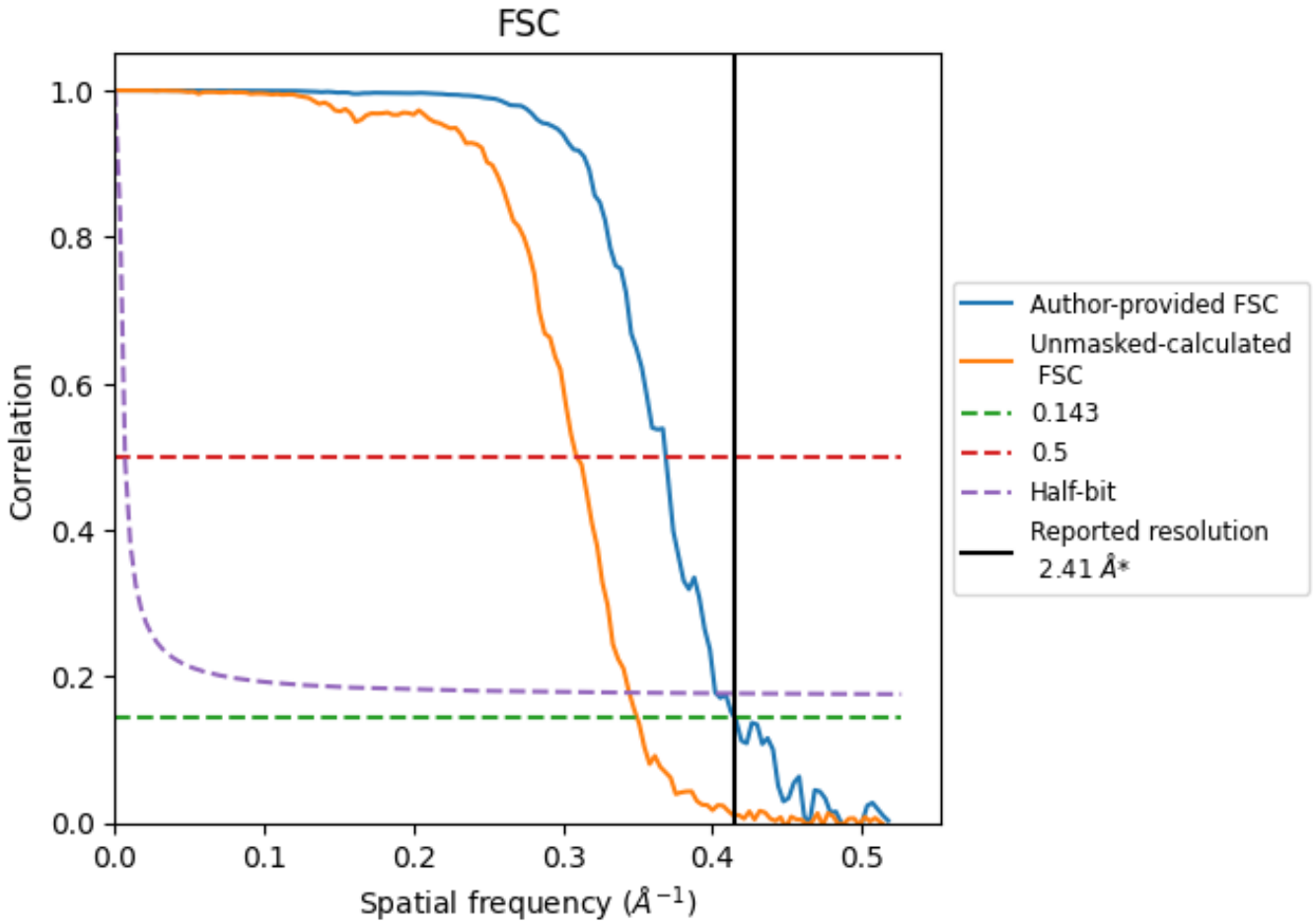


*Reported resolution corresponds to spatial frequency of 0.415 Å^{-1}

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 0.415 Å^{-1}

8.2 Resolution estimates (i)

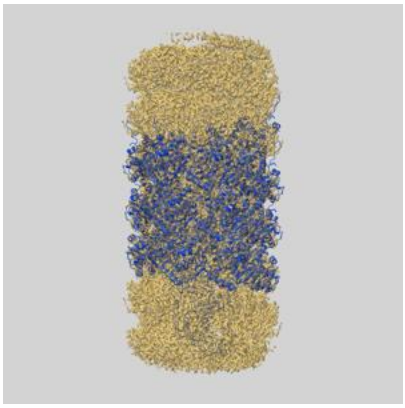
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.41	-	-
Author-provided FSC curve	2.41	2.71	2.49
Unmasked-calculated*	2.86	3.24	2.91

*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 2.86 differs from the reported value 2.41 by more than 10 %

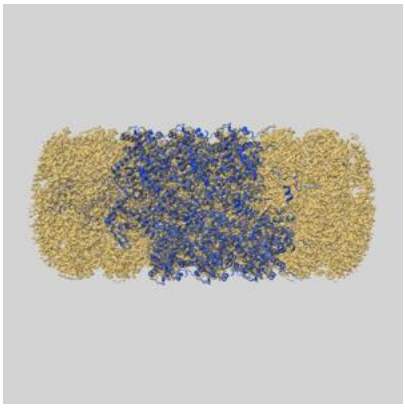
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17072 and PDB model 8OPL. Per-residue inclusion information can be found in section 3 on page 10.

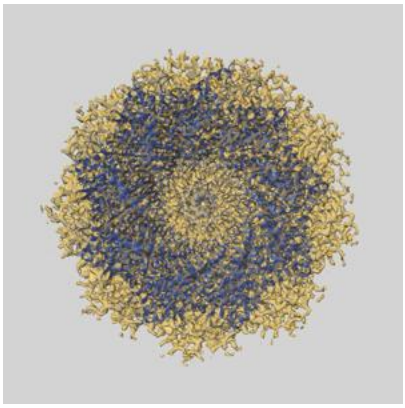
9.1 Map-model overlay



X



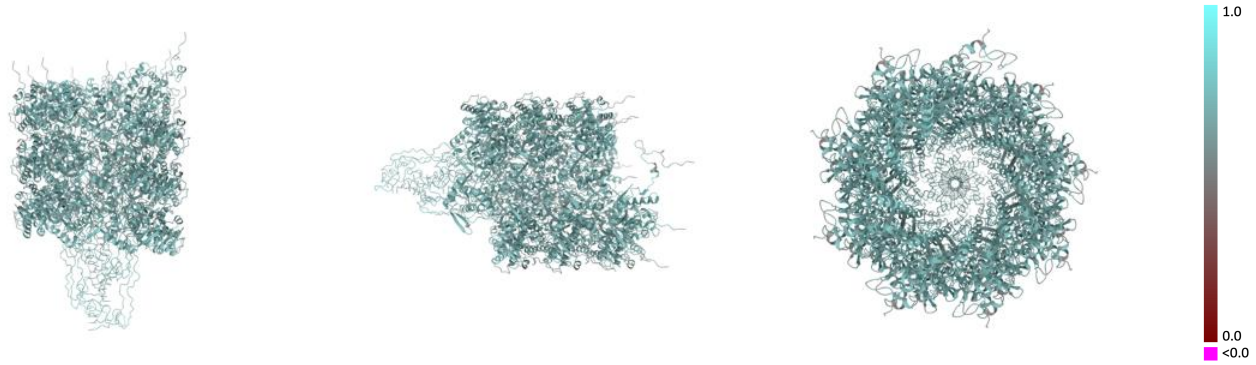
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.22 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.

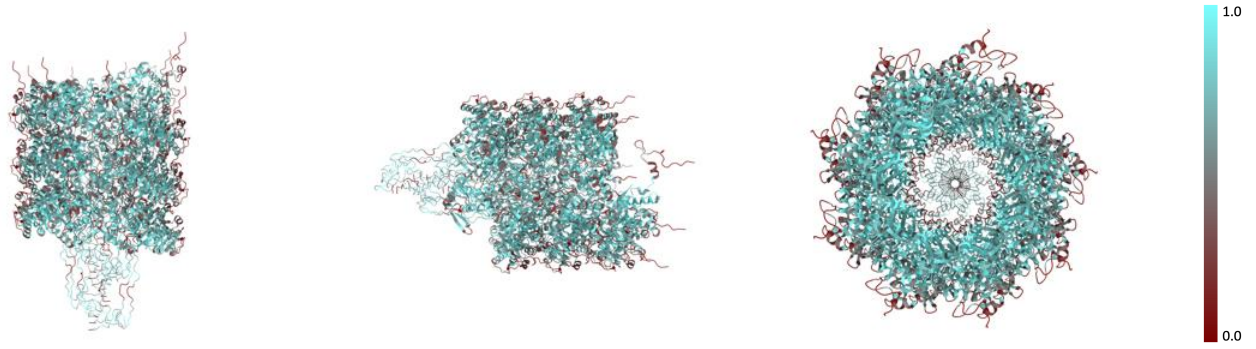
9.2 Q-score mapped to coordinate model (i)



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.

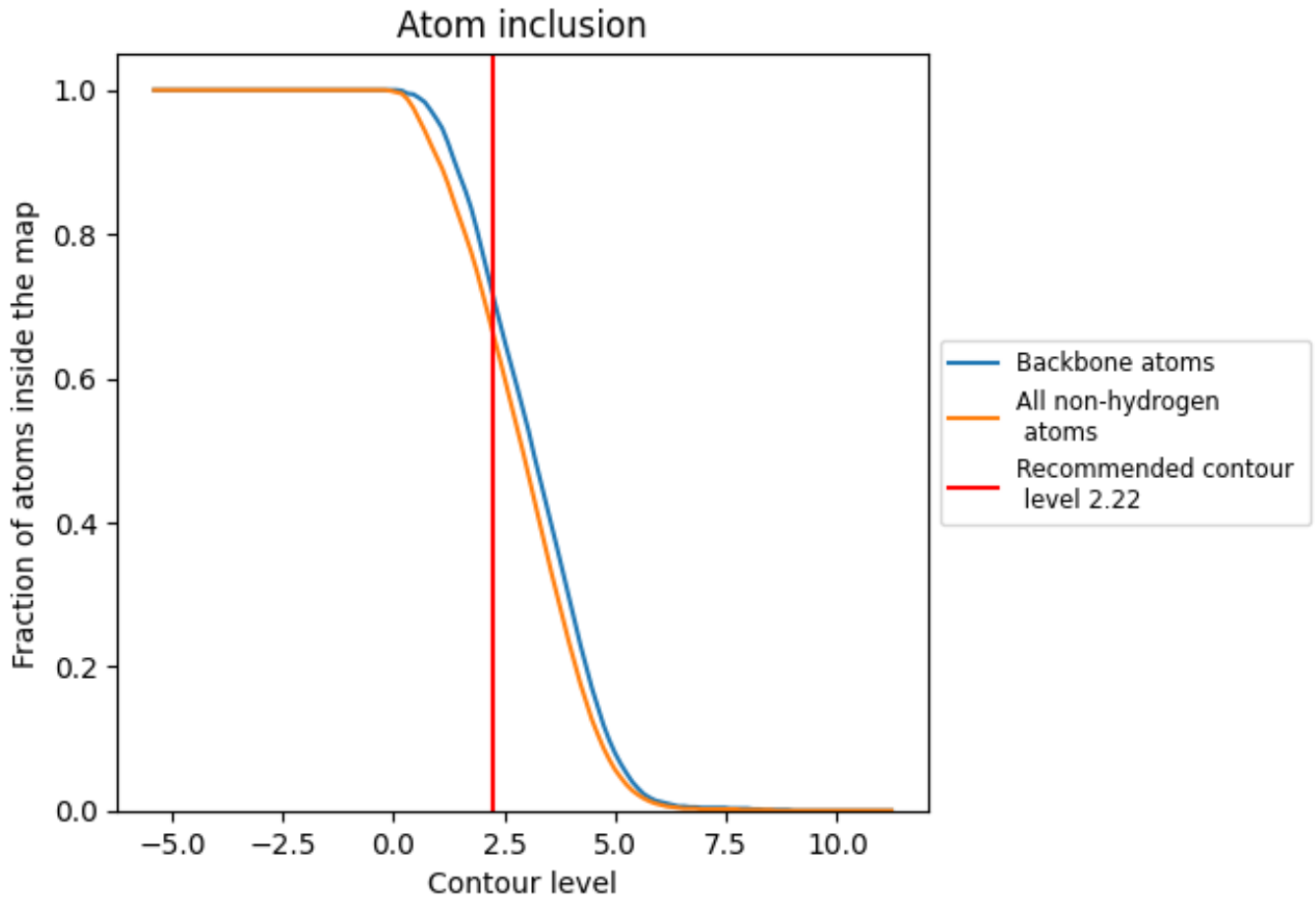
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.22).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6680	0.6670
Aa	0.6570	0.6680
Ab	0.6550	0.6670
Ac	0.6500	0.6680
Ad	0.6510	0.6670
Ae	0.6580	0.6670
Af	0.6560	0.6670
Ag	0.6570	0.6690
Ah	0.6580	0.6680
Ai	0.6540	0.6670
Aj	0.8300	0.6540
Ak	0.8600	0.6570
Al	0.8800	0.6520
Am	0.8700	0.6580
An	0.8600	0.6590
Ao	0.8800	0.6530
Ap	0.9000	0.6570
Aq	0.8600	0.6510
Ar	0.8900	0.6570
As	0.6520	0.6680
At	0.6680	0.6710
Au	0.6570	0.6670
Av	0.6530	0.6680
Aw	0.6570	0.6710
Ax	0.6610	0.6680
Ay	0.6570	0.6680
Az	0.6570	0.6690
Ba	0.6560	0.6670
Bb	0.8800	0.6530
Bc	0.8900	0.6480
Bd	0.8800	0.6490
Be	0.8700	0.6560
Bf	0.8700	0.6530
Bg	0.8800	0.6540
Bh	0.8900	0.6500

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Continued from previous page...

Chain	Atom inclusion	Q-score
Bi	0.8600	0.6550
Bj	0.8500	0.6520
Bk	0.6610	0.6660
Bl	0.6560	0.6660
Bm	0.6550	0.6680
Bn	0.6530	0.6660
Bo	0.6500	0.6650
Bp	0.6550	0.6680
Bq	0.6560	0.6660
Br	0.6630	0.6660
Bs	0.6600	0.6660
Bt	0.8900	0.6550
Bu	0.8800	0.6480
Bv	0.8600	0.6490
Bw	0.8600	0.6560
Bx	0.8500	0.6500
By	0.8600	0.6510
Bz	0.8900	0.6560
Ca	0.8800	0.6500
Cb	0.8600	0.6550