



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 07:15 am GMT

PDB ID : 8CO6
EMDB ID : EMD-16772
Title : Subtomogram average of Immature Rotavirus TLP penton
Authors : Shah, P.N.M.; Stuart, D.I.
Deposited on : 2023-02-27
Resolution : 4.70 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

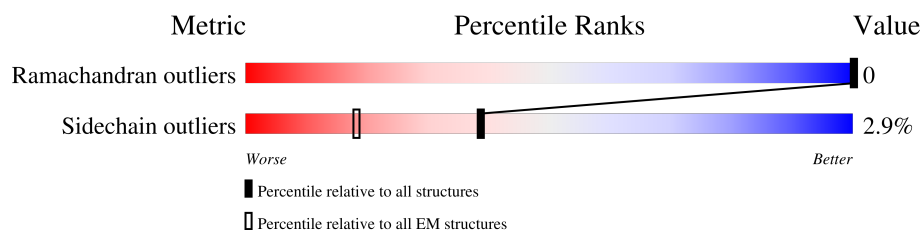
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 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	A	776	<div> <div>73%</div> <div>90%</div> <div>6%</div> </div>
1	B	776	<div> <div>77%</div> <div>94%</div> <div>.</div> </div>
1	C	776	<div> <div>52%</div> <div>87%</div> <div>11%</div> </div>
2	D	326	<div> <div>25%</div> <div>79%</div> <div>20%</div> </div>
2	E	326	<div> <div>62%</div> <div>73%</div> <div>25%</div> </div>
2	F	326	<div> <div>43%</div> <div>80%</div> <div>18%</div> </div>
2	G	326	<div> <div>45%</div> <div>81%</div> <div>18%</div> </div>
2	H	326	<div> <div>63%</div> <div>72%</div> <div>26%</div> </div>
2	I	326	<div> <div>30%</div> <div>79%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	326	
2	K	326	
2	L	326	
2	M	326	
2	N	326	
2	O	326	
3	d	397	
3	e	397	
3	f	397	
3	g	397	
3	h	397	
3	i	397	
3	j	397	
3	k	397	
3	l	397	
3	m	397	
3	n	397	
3	o	397	
4	q	882	
4	r	882	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 92540 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 Outer capsid protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	726	Total	C	N	O	S	0	0
			5715	3616	952	1128	19		
1	B	744	Total	C	N	O	S	0	0
			5860	3703	977	1160	20		
1	C	692	Total	C	N	O	S	0	0
			5478	3472	911	1075	20		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	THR	ARG	conflict	UNP A0A1Q2TSK9
A	323	MET	VAL	conflict	UNP A0A1Q2TSK9
A	737	SER	THR	conflict	UNP A0A1Q2TSK9
A	738	ARG	LYS	conflict	UNP A0A1Q2TSK9
B	185	THR	ARG	conflict	UNP A0A1Q2TSK9
B	323	MET	VAL	conflict	UNP A0A1Q2TSK9
B	737	SER	THR	conflict	UNP A0A1Q2TSK9
B	738	ARG	LYS	conflict	UNP A0A1Q2TSK9
C	185	THR	ARG	conflict	UNP A0A1Q2TSK9
C	323	MET	VAL	conflict	UNP A0A1Q2TSK9
C	737	SER	THR	conflict	UNP A0A1Q2TSK9
C	738	ARG	LYS	conflict	UNP A0A1Q2TSK9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	262	Total	C	N	O	S	0	0
			2077	1324	329	408	16		
2	E	244	Total	C	N	O	S	0	0
			1928	1227	304	381	16		
2	F	267	Total	C	N	O	S	0	0
			2118	1348	337	417	16		
2	G	268	Total	C	N	O	S	0	0
			2126	1354	338	418	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	242	Total	C	N	O	S	0	0
			1913	1217	302	378	16		
2	I	264	Total	C	N	O	S	0	0
			2096	1333	334	413	16		
2	J	265	Total	C	N	O	S	0	0
			2101	1336	335	414	16		
2	K	256	Total	C	N	O	S	0	0
			2031	1293	323	399	16		
2	L	265	Total	C	N	O	S	0	0
			2101	1336	335	414	16		
2	M	267	Total	C	N	O	S	0	0
			2118	1348	337	417	16		
2	N	263	Total	C	N	O	S	0	0
			2088	1329	333	410	16		
2	O	265	Total	C	N	O	S	0	0
			2101	1336	335	414	16		

- Molecule 3 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	e	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	f	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	g	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	h	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	i	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	j	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	k	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	l	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	m	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		
3	n	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	o	397	Total	C	N	O	S	0	0
			3163	2007	550	592	14		

- Molecule 4 is a protein called Inner capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	q	769	Total	C	N	O	S	0	0
			6254	3981	1072	1165	36		
4	r	795	Total	C	N	O	S	0	0
			6479	4125	1108	1210	36		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	118	ALA	LYS	conflict	UNP A2T3R1
q	129	ARG	LYS	conflict	UNP A2T3R1
q	131	LYS	LEU	conflict	UNP A2T3R1
q	135	ILE	ARG	conflict	UNP A2T3R1
q	140	LYS	ARG	conflict	UNP A2T3R1
q	142	ARG	LEU	conflict	UNP A2T3R1
q	146	ILE	TRP	conflict	UNP A2T3R1
q	152	LYS	ARG	conflict	UNP A2T3R1
q	175	THR	MET	conflict	UNP A2T3R1
q	206	SER	ALA	conflict	UNP A2T3R1
q	222	ALA	ARG	conflict	UNP A2T3R1
q	250	TYR	HIS	conflict	UNP A2T3R1
q	414	VAL	ILE	conflict	UNP A2T3R1
q	432	VAL	ILE	conflict	UNP A2T3R1
q	436	ILE	VAL	conflict	UNP A2T3R1
q	438	VAL	PRO	conflict	UNP A2T3R1
q	477	ASN	TYR	conflict	UNP A2T3R1
q	479	TYR	GLN	conflict	UNP A2T3R1
q	503	ILE	VAL	conflict	UNP A2T3R1
q	551	ALA	SER	conflict	UNP A2T3R1
q	553	SER	ASN	conflict	UNP A2T3R1
q	561	VAL	ILE	conflict	UNP A2T3R1
q	640	ALA	SER	conflict	UNP A2T3R1
q	650	HIS	GLN	conflict	UNP A2T3R1
q	656	VAL	ARG	conflict	UNP A2T3R1
q	657	ALA	VAL	conflict	UNP A2T3R1
q	676	VAL	ILE	conflict	UNP A2T3R1
q	686	LEU	ALA	conflict	UNP A2T3R1

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Chain	Residue	Modelled	Actual	Comment	Reference
q	688	ALA	ASN	conflict	UNP A2T3R1
q	690	ASP	GLU	conflict	UNP A2T3R1
q	741	THR	SER	conflict	UNP A2T3R1
q	743	SER	ASP	conflict	UNP A2T3R1
q	766	VAL	ILE	conflict	UNP A2T3R1
q	777	ILE	LYS	conflict	UNP A2T3R1
q	818	VAL	ILE	conflict	UNP A2T3R1
q	820	ILE	THR	conflict	UNP A2T3R1
q	831	VAL	GLN	conflict	UNP A2T3R1
q	837	ASN	ALA	conflict	UNP A2T3R1
r	118	ALA	LYS	conflict	UNP A2T3R1
r	129	ARG	LYS	conflict	UNP A2T3R1
r	131	LYS	LEU	conflict	UNP A2T3R1
r	135	ILE	ARG	conflict	UNP A2T3R1
r	140	LYS	ARG	conflict	UNP A2T3R1
r	142	ARG	LEU	conflict	UNP A2T3R1
r	146	ILE	TRP	conflict	UNP A2T3R1
r	152	LYS	ARG	conflict	UNP A2T3R1
r	175	THR	MET	conflict	UNP A2T3R1
r	206	SER	ALA	conflict	UNP A2T3R1
r	222	ALA	ARG	conflict	UNP A2T3R1
r	250	TYR	HIS	conflict	UNP A2T3R1
r	414	VAL	ILE	conflict	UNP A2T3R1
r	432	VAL	ILE	conflict	UNP A2T3R1
r	436	ILE	VAL	conflict	UNP A2T3R1
r	438	VAL	PRO	conflict	UNP A2T3R1
r	477	ASN	TYR	conflict	UNP A2T3R1
r	479	TYR	GLN	conflict	UNP A2T3R1
r	503	ILE	VAL	conflict	UNP A2T3R1
r	551	ALA	SER	conflict	UNP A2T3R1
r	553	SER	ASN	conflict	UNP A2T3R1
r	561	VAL	ILE	conflict	UNP A2T3R1
r	640	ALA	SER	conflict	UNP A2T3R1
r	650	HIS	GLN	conflict	UNP A2T3R1
r	656	VAL	ARG	conflict	UNP A2T3R1
r	657	ALA	VAL	conflict	UNP A2T3R1
r	676	VAL	ILE	conflict	UNP A2T3R1
r	686	LEU	ALA	conflict	UNP A2T3R1
r	688	ALA	ASN	conflict	UNP A2T3R1
r	690	ASP	GLU	conflict	UNP A2T3R1
r	741	THR	SER	conflict	UNP A2T3R1
r	743	SER	ASP	conflict	UNP A2T3R1

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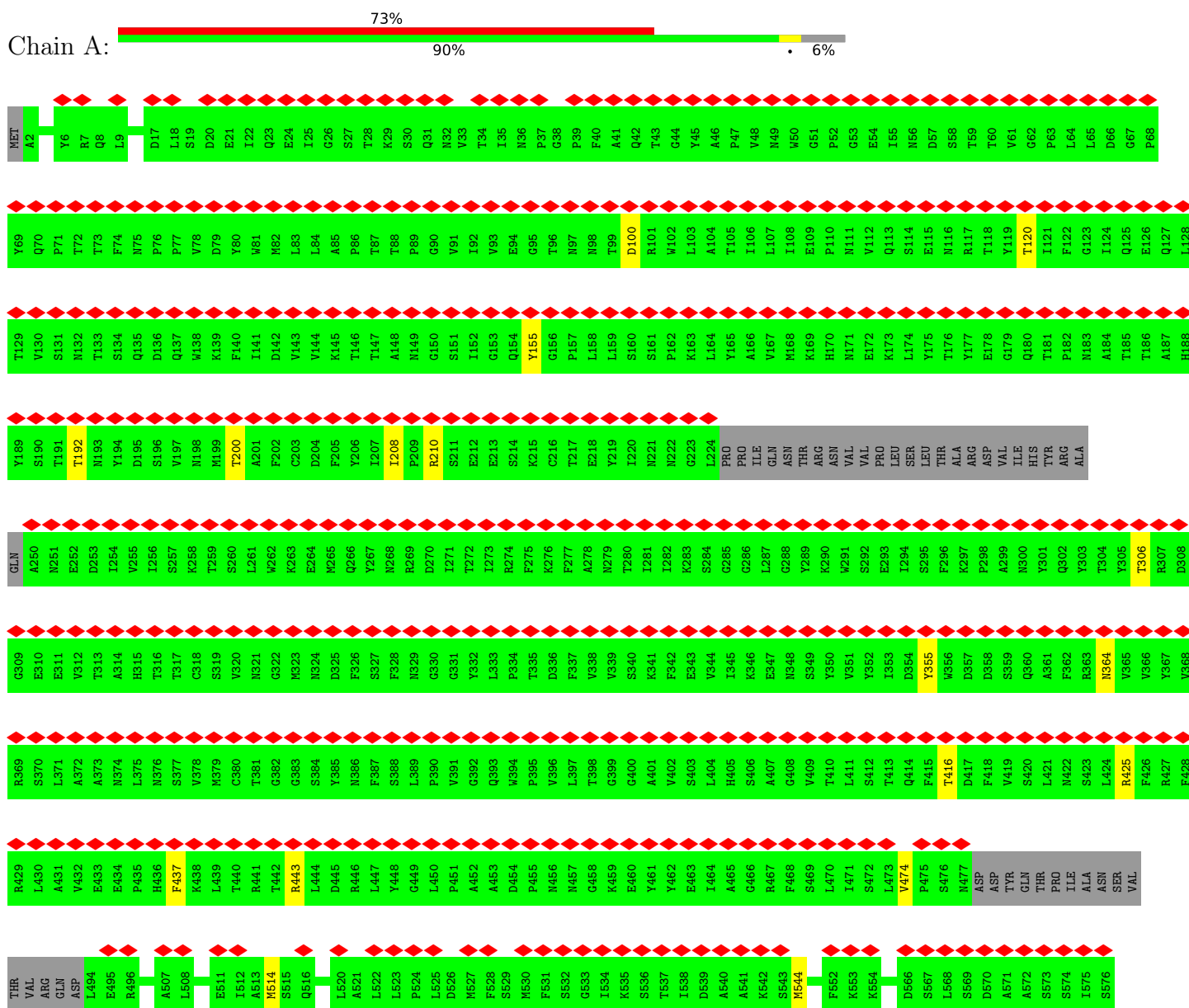
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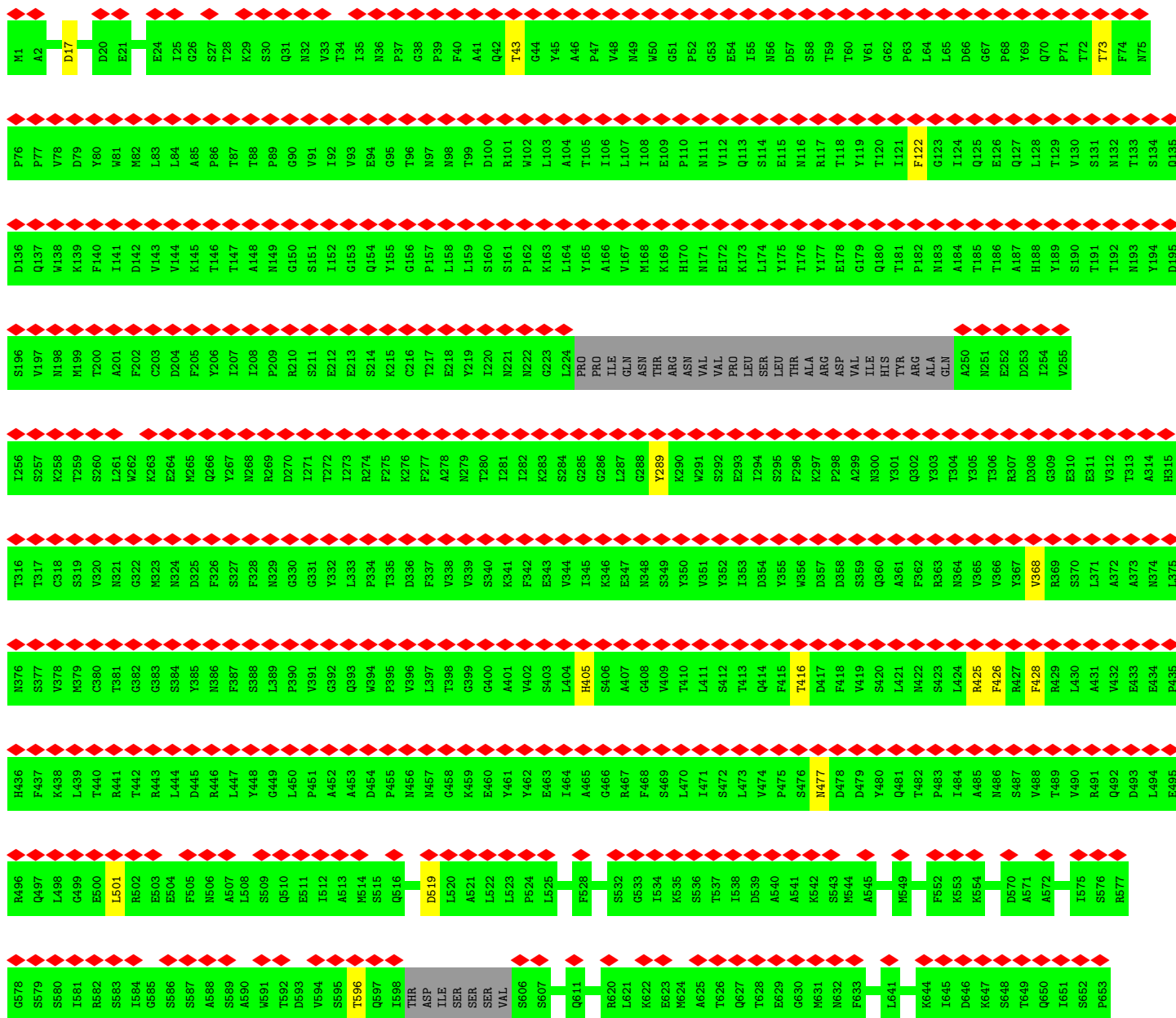
Chain	Residue	Modelled	Actual	Comment	Reference
r	766	VAL	ILE	conflict	UNP A2T3R1
r	777	ILE	LYS	conflict	UNP A2T3R1
r	818	VAL	ILE	conflict	UNP A2T3R1
r	820	ILE	THR	conflict	UNP A2T3R1
r	831	VAL	GLN	conflict	UNP A2T3R1
r	837	ASN	ALA	conflict	UNP A2T3R1

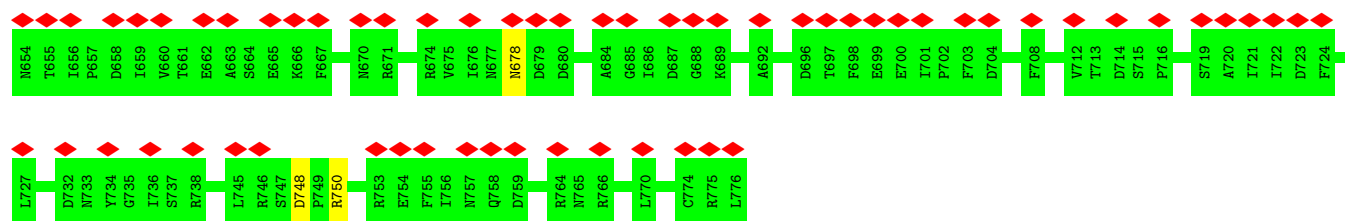
3 Residue-property plots

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

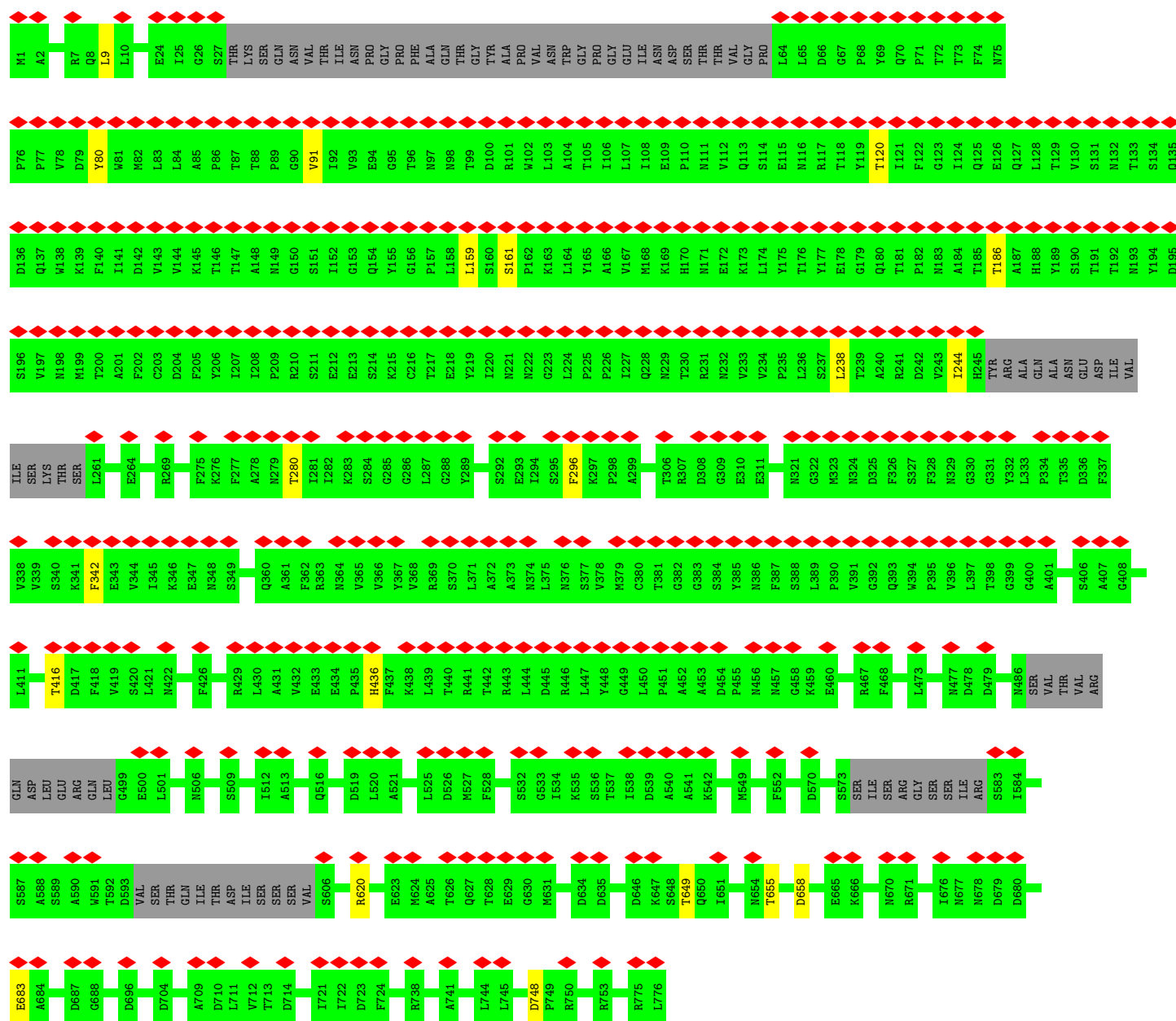
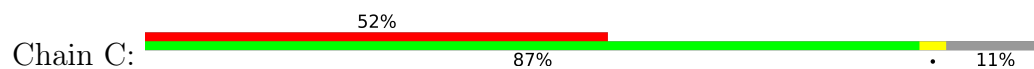
• Molecule 1: Outer capsid protein VP4



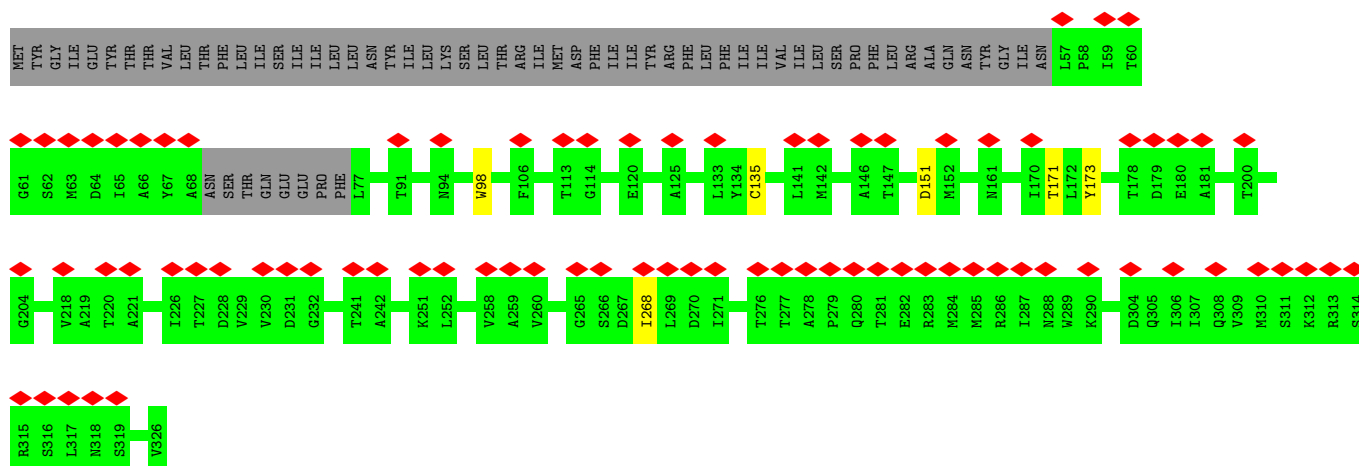
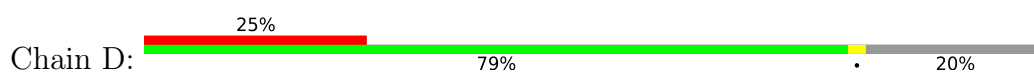




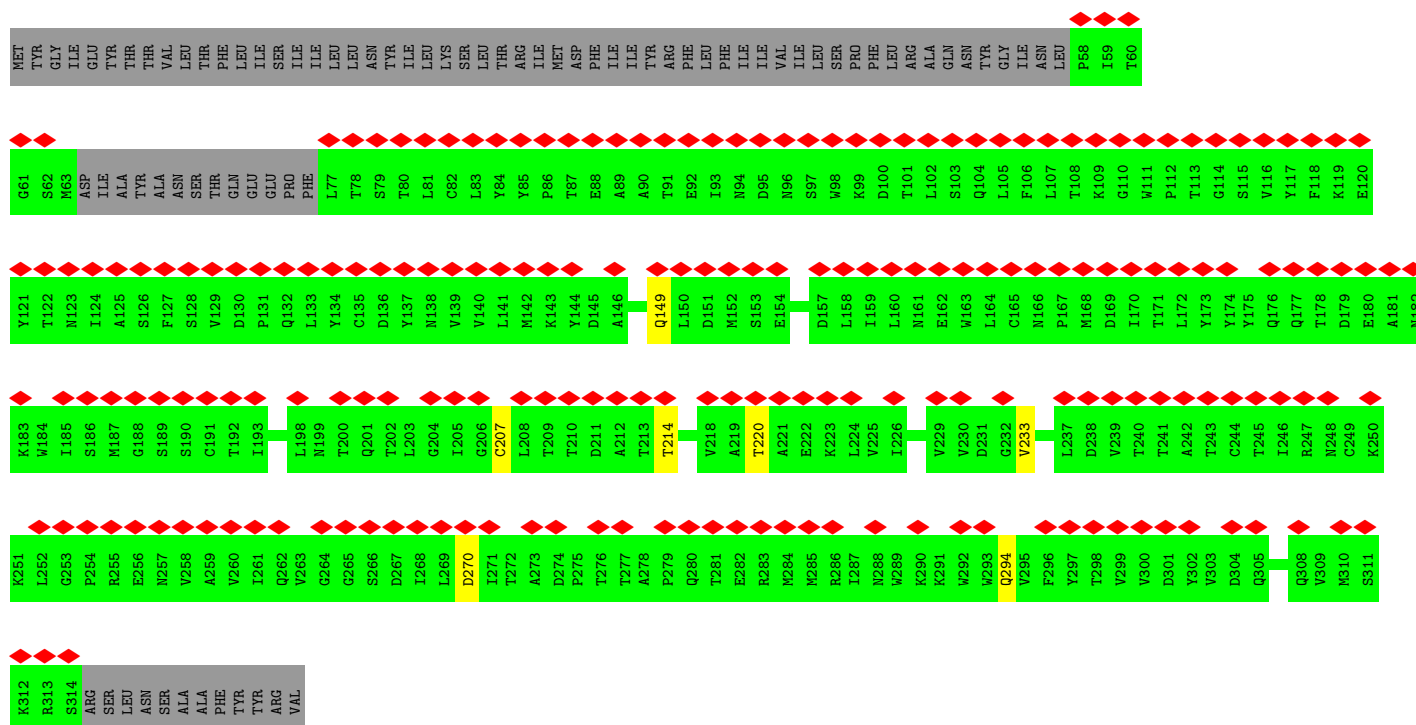
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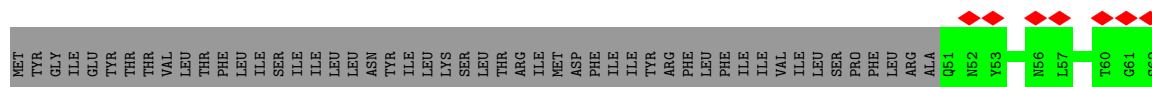
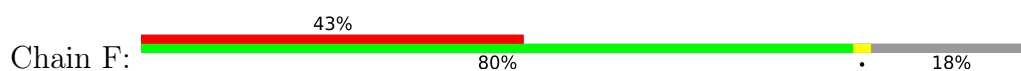
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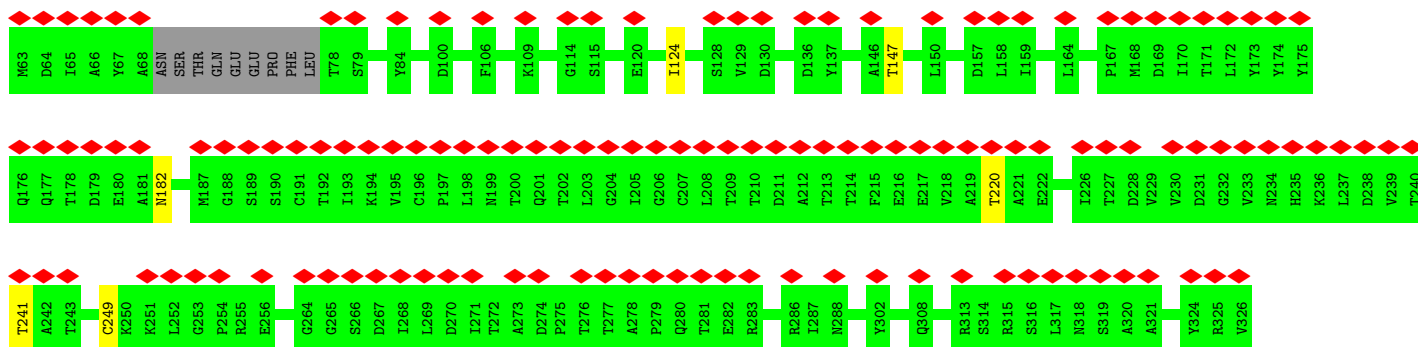


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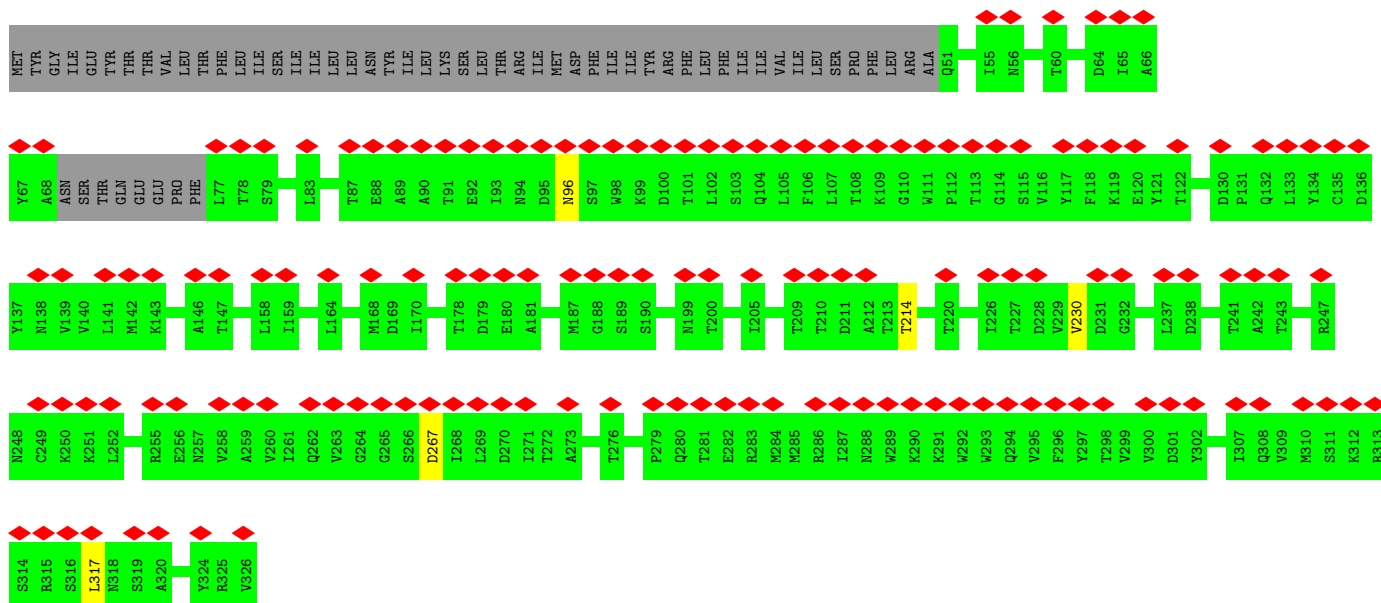
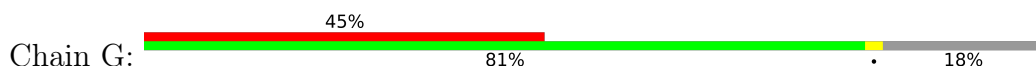


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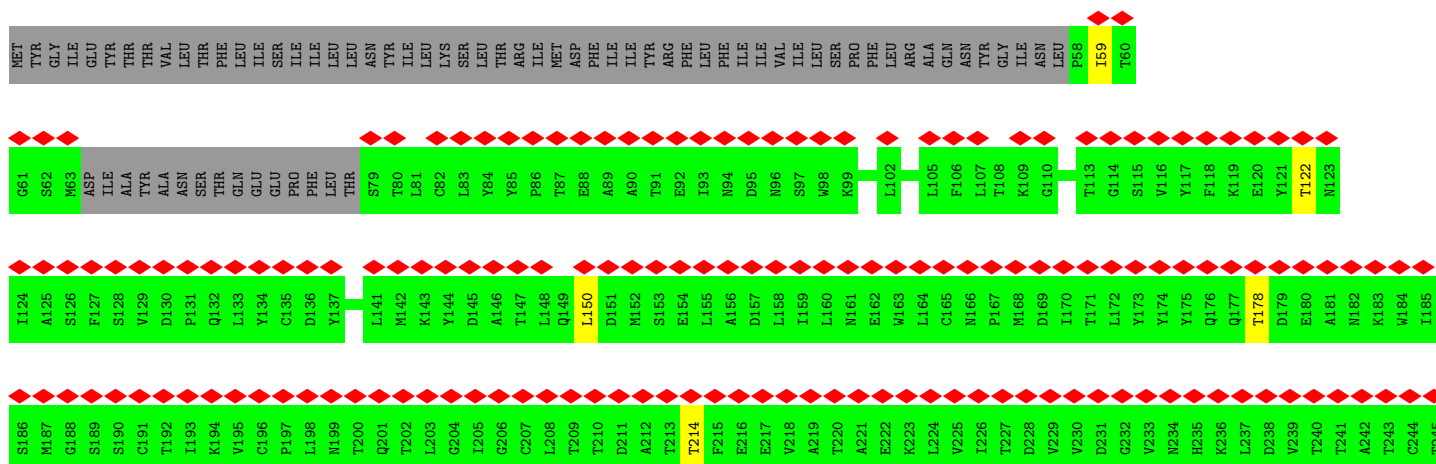
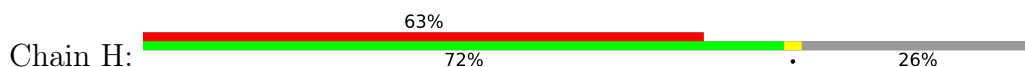




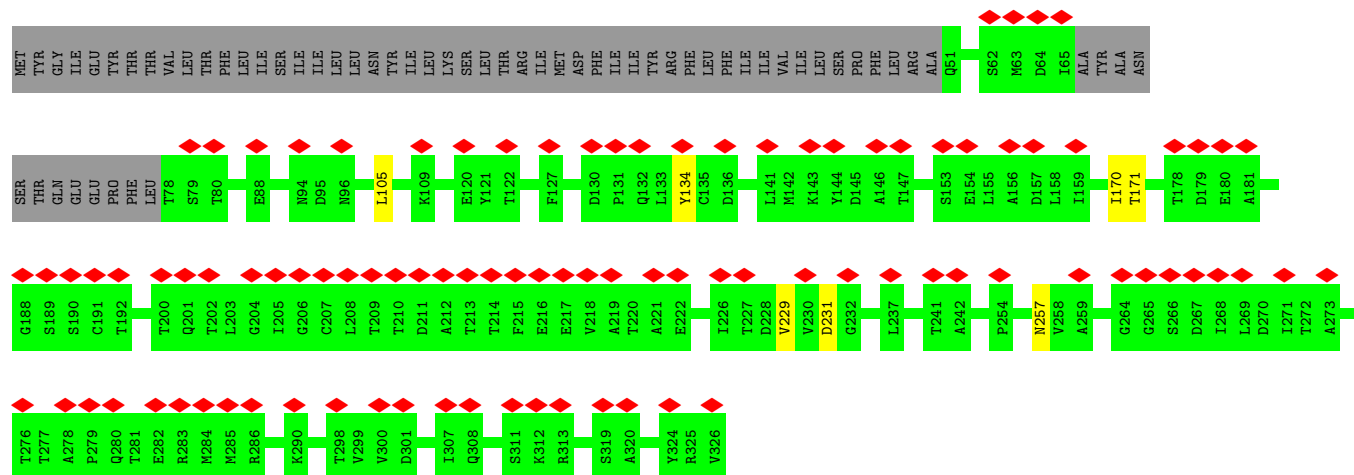
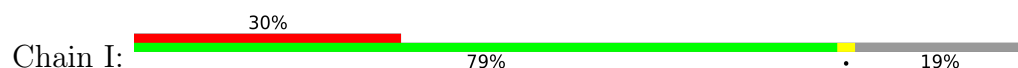
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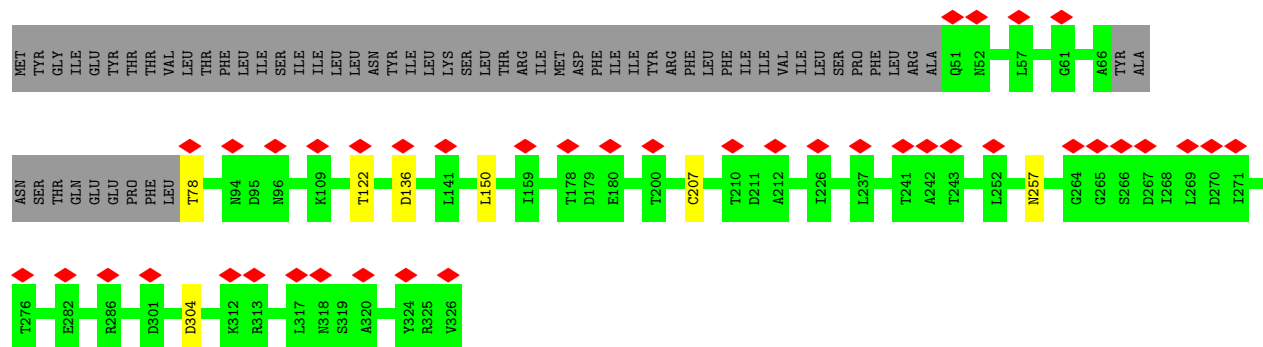
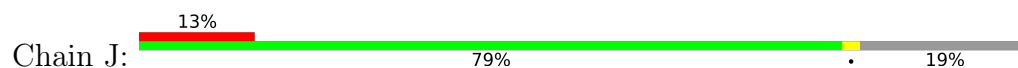
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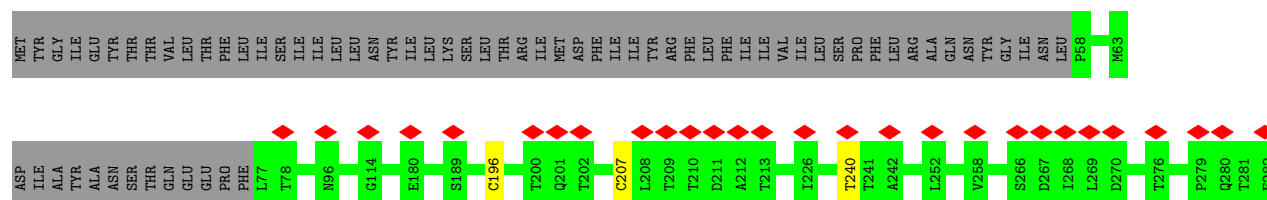
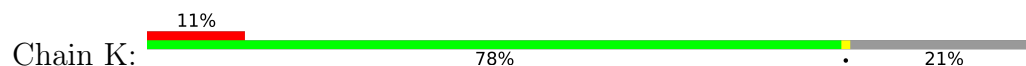
- Molecule 2: Outer capsid glycoprotein VP7

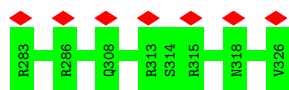


- Molecule 2: Outer capsid glycoprotein VP7

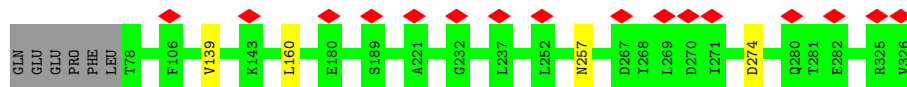
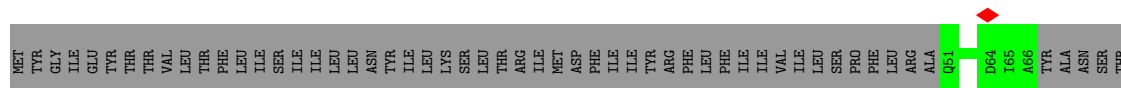
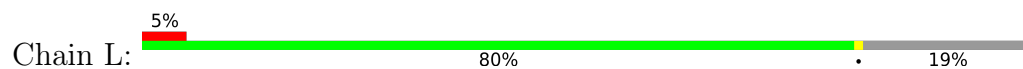


- Molecule 2: Outer capsid glycoprotein VP7

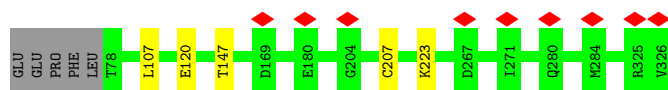
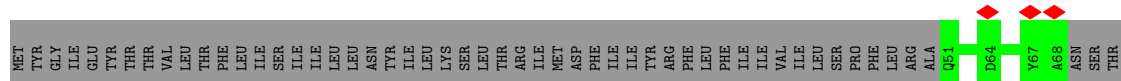
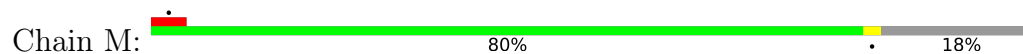




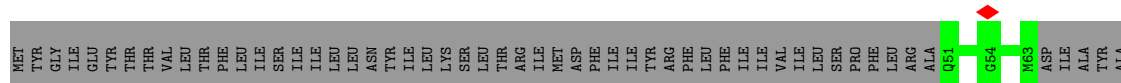
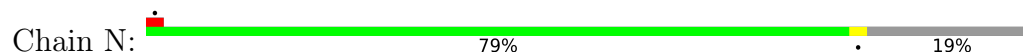
- Molecule 2: Outer capsid glycoprotein VP7



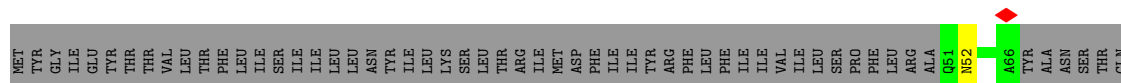
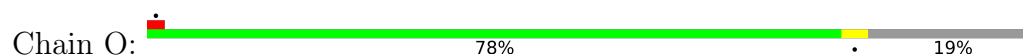
- Molecule 2: Outer capsid glycoprotein VP7



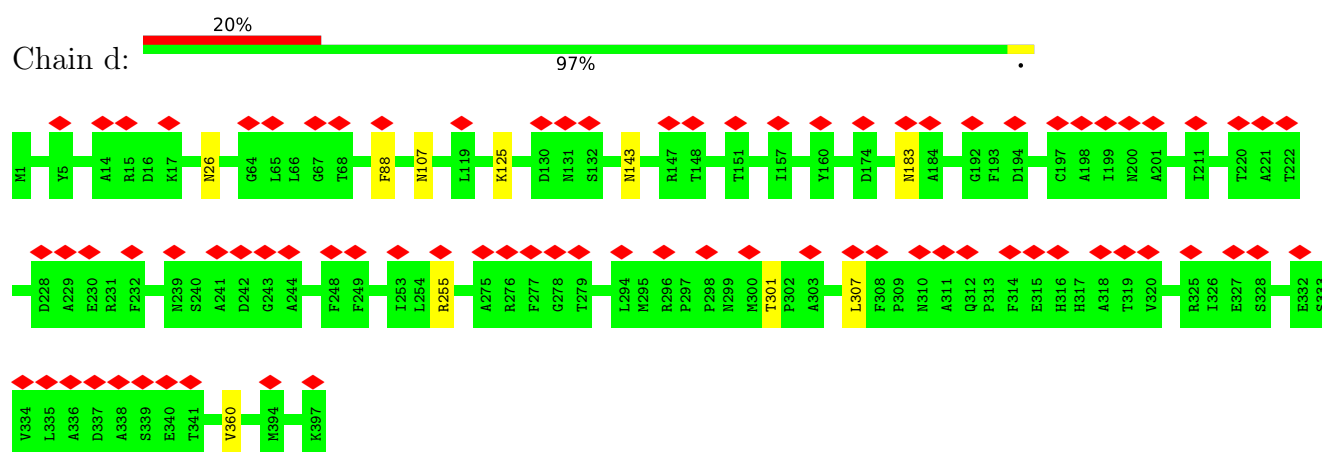
- Molecule 2: Outer capsid glycoprotein VP7



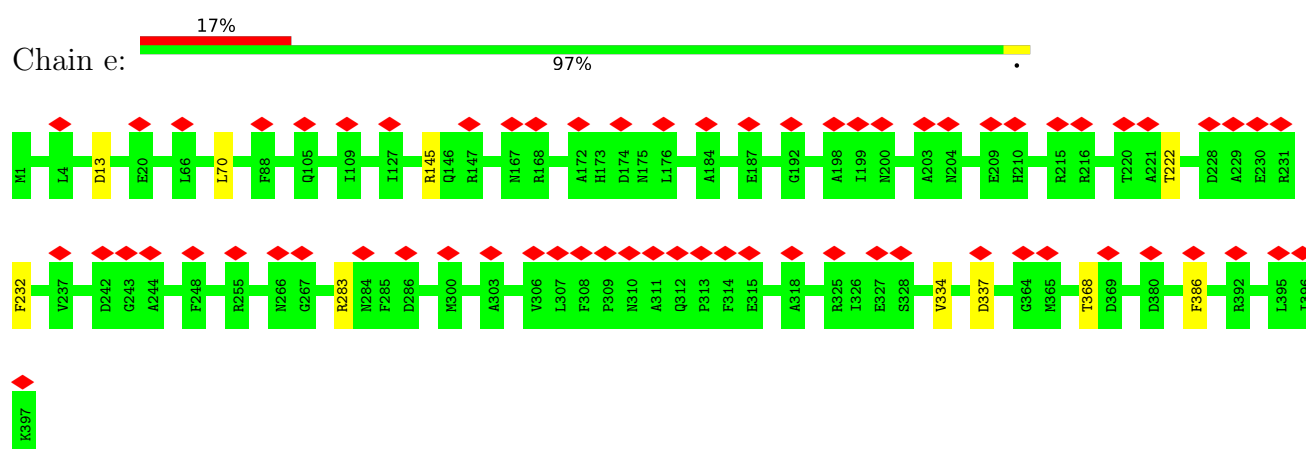
- Molecule 2: Outer capsid glycoprotein VP7



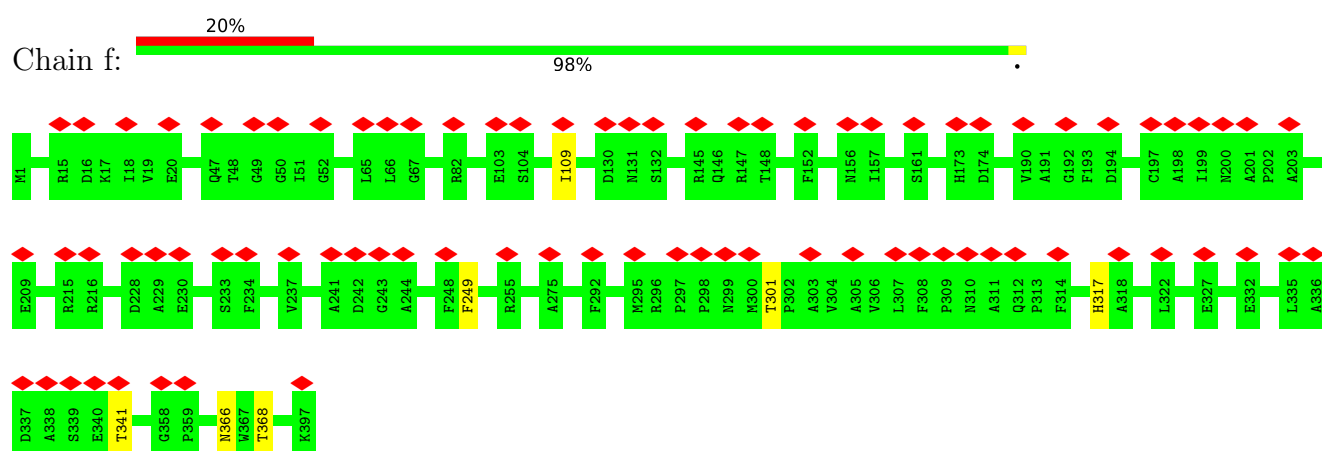
- Molecule 3: Intermediate capsid protein VP6



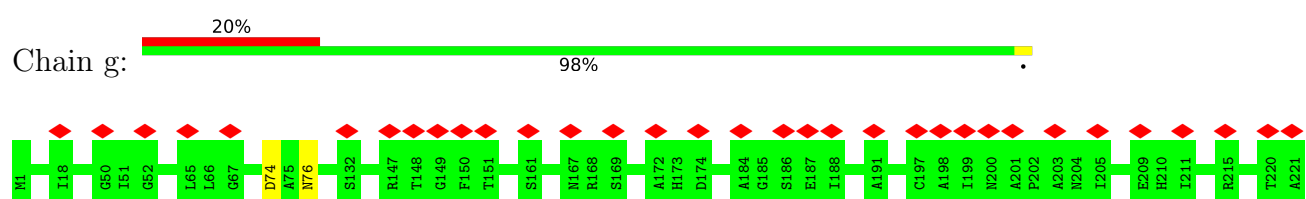
• Molecule 3: Intermediate capsid protein VP6

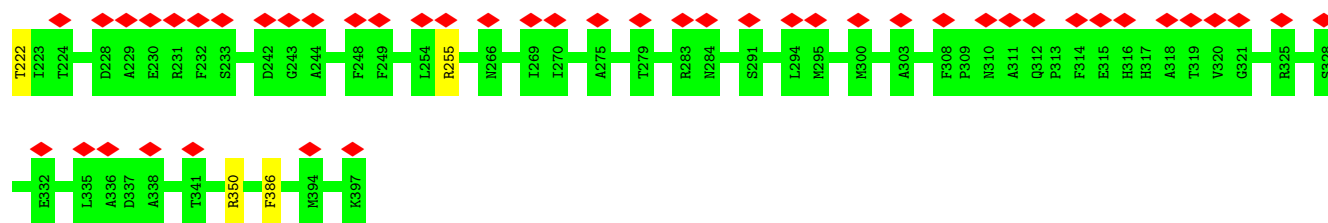


• Molecule 3: Intermediate capsid protein VP6

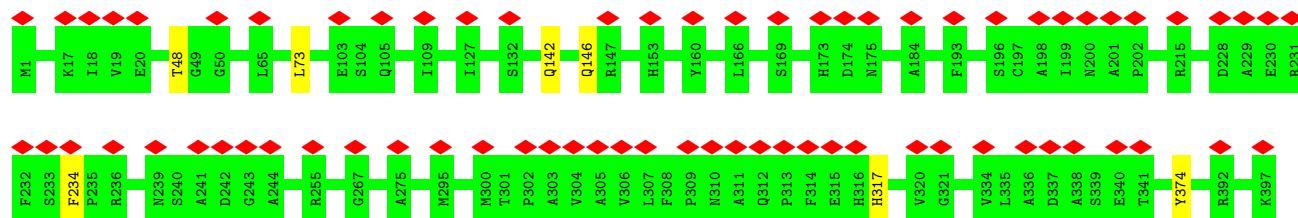


• Molecule 3: Intermediate capsid protein VP6

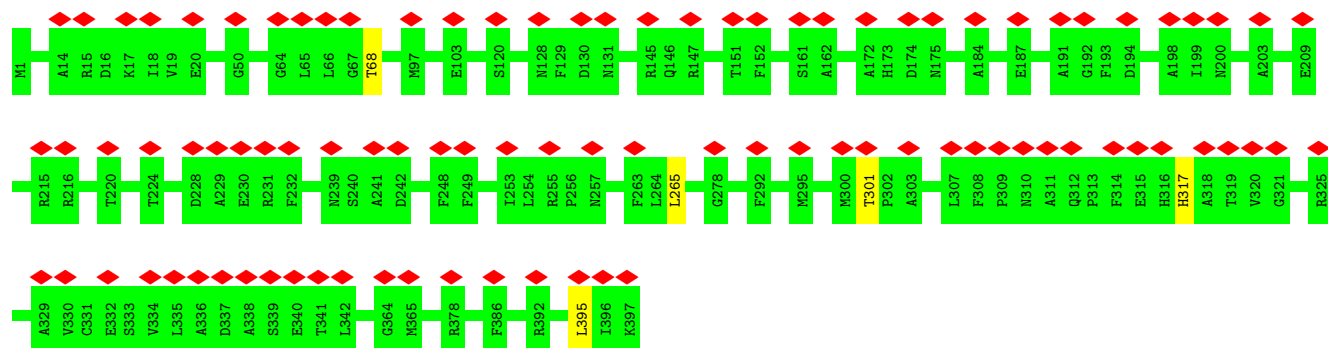




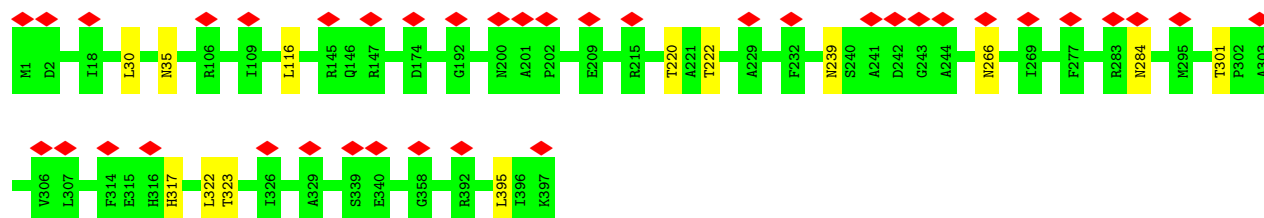
• Molecule 3: Intermediate capsid protein VP6



• Molecule 3: Intermediate capsid protein VP6

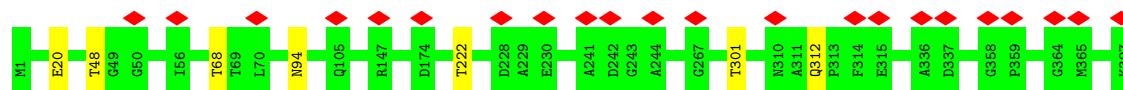


• Molecule 3: Intermediate capsid protein VP6

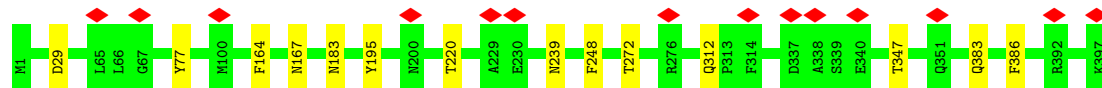


• Molecule 3: Intermediate capsid protein VP6

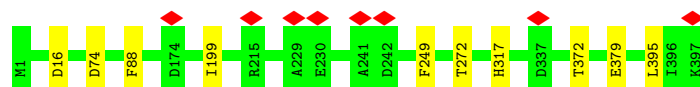




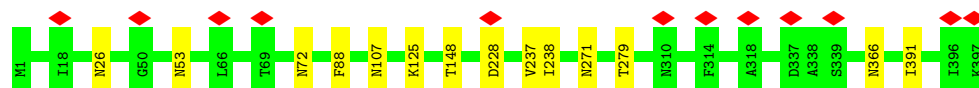
• Molecule 3: Intermediate capsid protein VP6



• Molecule 3: Intermediate capsid protein VP6



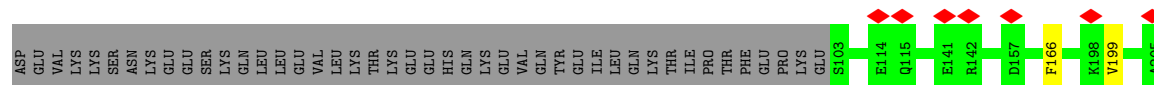
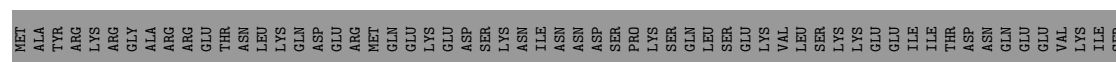
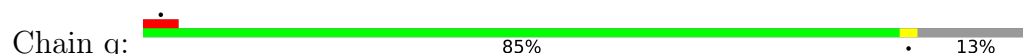
• Molecule 3: Intermediate capsid protein VP6

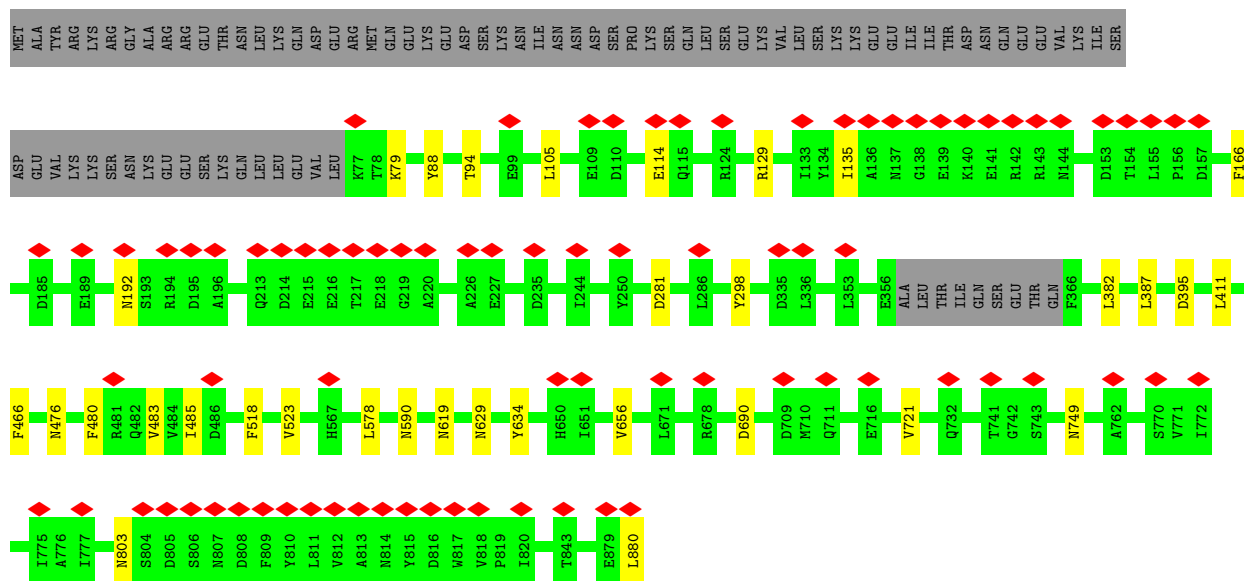


• Molecule 3: Intermediate capsid protein VP6



• Molecule 4: Inner capsid protein VP2





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of subtomograms used	1961	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 ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.009	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	413.7, 413.7, 413.7	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.97, 1.97, 1.97	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/5833	0.47	0/7925
1	B	0.24	0/5981	0.47	0/8129
1	C	0.25	0/5591	0.46	0/7594
2	D	0.24	0/2120	0.46	0/2893
2	E	0.24	0/1967	0.44	0/2685
2	F	0.24	0/2162	0.46	0/2950
2	G	0.24	0/2170	0.47	0/2961
2	H	0.23	0/1952	0.45	0/2664
2	I	0.25	0/2139	0.46	0/2918
2	J	0.24	0/2144	0.45	0/2925
2	K	0.24	0/2073	0.46	0/2827
2	L	0.25	0/2144	0.45	0/2925
2	M	0.26	0/2162	0.47	0/2950
2	N	0.25	0/2131	0.46	0/2907
2	O	0.25	0/2144	0.46	0/2925
3	d	0.25	0/3234	0.47	0/4402
3	e	0.25	0/3234	0.49	0/4402
3	f	0.25	0/3234	0.49	0/4402
3	g	0.25	0/3234	0.48	0/4402
3	h	0.25	0/3234	0.48	0/4402
3	i	0.25	0/3234	0.48	0/4402
3	j	0.25	0/3234	0.48	0/4402
3	k	0.26	0/3234	0.48	0/4402
3	l	0.26	0/3234	0.49	0/4402
3	m	0.26	0/3234	0.49	0/4402
3	n	0.27	0/3234	0.49	0/4402
3	o	0.26	0/3234	0.49	0/4402
4	q	0.25	0/6367	0.46	0/8639
4	r	0.25	0/6597	0.46	0/8948
All	All	0.25	0/94485	0.47	0/128589

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	A	718/776 (92%)	680 (95%)	38 (5%)	0	100	100
1	B	738/776 (95%)	695 (94%)	43 (6%)	0	100	100
1	C	680/776 (88%)	640 (94%)	40 (6%)	0	100	100
2	D	258/326 (79%)	246 (95%)	12 (5%)	0	100	100
2	E	240/326 (74%)	232 (97%)	8 (3%)	0	100	100
2	F	263/326 (81%)	253 (96%)	10 (4%)	0	100	100
2	G	264/326 (81%)	253 (96%)	11 (4%)	0	100	100
2	H	238/326 (73%)	228 (96%)	10 (4%)	0	100	100
2	I	260/326 (80%)	248 (95%)	12 (5%)	0	100	100
2	J	261/326 (80%)	250 (96%)	11 (4%)	0	100	100
2	K	252/326 (77%)	243 (96%)	9 (4%)	0	100	100
2	L	261/326 (80%)	250 (96%)	11 (4%)	0	100	100
2	M	263/326 (81%)	245 (93%)	18 (7%)	0	100	100
2	N	259/326 (79%)	237 (92%)	22 (8%)	0	100	100
2	O	261/326 (80%)	239 (92%)	22 (8%)	0	100	100
3	d	395/397 (100%)	385 (98%)	10 (2%)	0	100	100
3	e	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	f	395/397 (100%)	381 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	395/397 (100%)	377 (95%)	18 (5%)	0	100	100
3	h	395/397 (100%)	381 (96%)	14 (4%)	0	100	100
3	i	395/397 (100%)	382 (97%)	13 (3%)	0	100	100
3	j	395/397 (100%)	376 (95%)	19 (5%)	0	100	100
3	k	395/397 (100%)	377 (95%)	18 (5%)	0	100	100
3	l	395/397 (100%)	381 (96%)	14 (4%)	0	100	100
3	m	395/397 (100%)	372 (94%)	23 (6%)	0	100	100
3	n	395/397 (100%)	379 (96%)	16 (4%)	0	100	100
3	o	395/397 (100%)	370 (94%)	25 (6%)	0	100	100
4	q	765/882 (87%)	734 (96%)	31 (4%)	0	100	100
4	r	791/882 (90%)	756 (96%)	35 (4%)	0	100	100
All	All	11512/12768 (90%)	10970 (95%)	542 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	642/689 (93%)	617 (96%)	25 (4%)	27	49
1	B	659/689 (96%)	641 (97%)	18 (3%)	40	60
1	C	615/689 (89%)	595 (97%)	20 (3%)	33	54
2	D	235/296 (79%)	229 (97%)	6 (3%)	41	61
2	E	221/296 (75%)	214 (97%)	7 (3%)	34	54
2	F	239/296 (81%)	233 (98%)	6 (2%)	42	62
2	G	240/296 (81%)	235 (98%)	5 (2%)	48	67
2	H	219/296 (74%)	212 (97%)	7 (3%)	34	54
2	I	238/296 (80%)	231 (97%)	7 (3%)	37	58
2	J	238/296 (80%)	231 (97%)	7 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	231/296 (78%)	228 (99%)	3 (1%)	65	77
2	L	238/296 (80%)	234 (98%)	4 (2%)	56	73
2	M	239/296 (81%)	234 (98%)	5 (2%)	48	67
2	N	237/296 (80%)	230 (97%)	7 (3%)	36	56
2	O	238/296 (80%)	228 (96%)	10 (4%)	25	47
3	d	351/351 (100%)	341 (97%)	10 (3%)	38	59
3	e	351/351 (100%)	341 (97%)	10 (3%)	38	59
3	f	351/351 (100%)	344 (98%)	7 (2%)	50	69
3	g	351/351 (100%)	345 (98%)	6 (2%)	56	73
3	h	351/351 (100%)	344 (98%)	7 (2%)	50	69
3	i	351/351 (100%)	346 (99%)	5 (1%)	62	76
3	j	351/351 (100%)	338 (96%)	13 (4%)	29	51
3	k	351/351 (100%)	344 (98%)	7 (2%)	50	69
3	l	351/351 (100%)	337 (96%)	14 (4%)	27	48
3	m	351/351 (100%)	341 (97%)	10 (3%)	38	59
3	n	351/351 (100%)	337 (96%)	14 (4%)	27	48
3	o	351/351 (100%)	342 (97%)	9 (3%)	41	61
4	q	700/809 (86%)	680 (97%)	20 (3%)	37	58
4	r	726/809 (90%)	693 (96%)	33 (4%)	23	46
All	All	10367/11449 (90%)	10065 (97%)	302 (3%)	39	58

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	120	THR
1	A	155	TYR
1	A	192	THR
1	A	200	THR
1	A	208	ILE
1	A	210	ARG
1	A	306	THR
1	A	355	TYR
1	A	364	ASN
1	A	416	THR

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Mol	Chain	Res	Type
1	A	425	ARG
1	A	437	PHE
1	A	443	ARG
1	A	474	VAL
1	A	514	MET
1	A	544	MET
1	A	592	THR
1	A	593	ASP
1	A	594	VAL
1	A	620	ARG
1	A	649	THR
1	A	655	THR
1	A	661	THR
1	A	757	ASN
1	B	17	ASP
1	B	43	THR
1	B	73	THR
1	B	122	PHE
1	B	289	TYR
1	B	368	VAL
1	B	405	HIS
1	B	416	THR
1	B	425	ARG
1	B	426	PHE
1	B	428	PHE
1	B	477	ASN
1	B	501	LEU
1	B	519	ASP
1	B	596	THR
1	B	678	ASN
1	B	748	ASP
1	B	750	ARG
1	C	9	LEU
1	C	80	TYR
1	C	91	VAL
1	C	120	THR
1	C	159	LEU
1	C	161	SER
1	C	186	THR
1	C	238	LEU
1	C	244	ILE
1	C	280	THR

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Mol	Chain	Res	Type
1	C	296	PHE
1	C	342	PHE
1	C	416	THR
1	C	436	HIS
1	C	620	ARG
1	C	649	THR
1	C	655	THR
1	C	658	ASP
1	C	683	GLU
1	C	748	ASP
2	D	98	TRP
2	D	135	CYS
2	D	151	ASP
2	D	171	THR
2	D	173	TYR
2	D	268	ILE
2	E	149	GLN
2	E	207	CYS
2	E	214	THR
2	E	220	THR
2	E	233	VAL
2	E	270	ASP
2	E	294	GLN
2	F	124	ILE
2	F	147	THR
2	F	182	ASN
2	F	220	THR
2	F	241	THR
2	F	249	CYS
2	G	96	ASN
2	G	214	THR
2	G	230	VAL
2	G	267	ASP
2	G	317	LEU
2	H	59	ILE
2	H	122	THR
2	H	150	LEU
2	H	178	THR
2	H	214	THR
2	H	289	TRP
2	H	309	VAL
2	I	105	LEU

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Mol	Chain	Res	Type
2	I	134	TYR
2	I	170	ILE
2	I	171	THR
2	I	229	VAL
2	I	231	ASP
2	I	257	ASN
2	J	78	THR
2	J	122	THR
2	J	136	ASP
2	J	150	LEU
2	J	207	CYS
2	J	257	ASN
2	J	304	ASP
2	K	196	CYS
2	K	207	CYS
2	K	240	THR
2	L	139	VAL
2	L	160	LEU
2	L	257	ASN
2	L	274	ASP
2	M	107	LEU
2	M	120	GLU
2	M	147	THR
2	M	207	CYS
2	M	223	LYS
2	N	154	GLU
2	N	155	LEU
2	N	207	CYS
2	N	229	VAL
2	N	240	THR
2	N	304	ASP
2	N	324	TYR
2	O	52	ASN
2	O	78	THR
2	O	135	CYS
2	O	147	THR
2	O	173	TYR
2	O	229	VAL
2	O	262	GLN
2	O	285	MET
2	O	296	PHE
2	O	323	TYR

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Mol	Chain	Res	Type
3	d	26	ASN
3	d	88	PHE
3	d	107	ASN
3	d	125	LYS
3	d	143	ASN
3	d	183	ASN
3	d	255	ARG
3	d	301	THR
3	d	307	LEU
3	d	360	VAL
3	e	13	ASP
3	e	70	LEU
3	e	145	ARG
3	e	222	THR
3	e	232	PHE
3	e	283	ARG
3	e	334	VAL
3	e	337	ASP
3	e	368	THR
3	e	386	PHE
3	f	109	ILE
3	f	249	PHE
3	f	301	THR
3	f	317	HIS
3	f	341	THR
3	f	366	ASN
3	f	368	THR
3	g	74	ASP
3	g	76	ASN
3	g	222	THR
3	g	255	ARG
3	g	350	ARG
3	g	386	PHE
3	h	48	THR
3	h	73	LEU
3	h	142	GLN
3	h	146	GLN
3	h	234	PHE
3	h	317	HIS
3	h	374	TYR
3	i	68	THR
3	i	265	LEU

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Mol	Chain	Res	Type
3	i	301	THR
3	i	317	HIS
3	i	395	LEU
3	j	30	LEU
3	j	35	ASN
3	j	116	LEU
3	j	220	THR
3	j	222	THR
3	j	239	ASN
3	j	266	ASN
3	j	284	ASN
3	j	301	THR
3	j	317	HIS
3	j	322	LEU
3	j	323	THR
3	j	395	LEU
3	k	20	GLU
3	k	48	THR
3	k	68	THR
3	k	94	ASN
3	k	222	THR
3	k	301	THR
3	k	312	GLN
3	l	29	ASP
3	l	77	TYR
3	l	164	PHE
3	l	167	ASN
3	l	183	ASN
3	l	195	TYR
3	l	220	THR
3	l	239	ASN
3	l	248	PHE
3	l	272	THR
3	l	312	GLN
3	l	347	THR
3	l	383	GLN
3	l	386	PHE
3	m	16	ASP
3	m	74	ASP
3	m	88	PHE
3	m	199	ILE
3	m	249	PHE

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Mol	Chain	Res	Type
3	m	272	THR
3	m	317	HIS
3	m	372	THR
3	m	379	GLU
3	m	395	LEU
3	n	26	ASN
3	n	53	ASN
3	n	72	ASN
3	n	88	PHE
3	n	107	ASN
3	n	125	LYS
3	n	148	THR
3	n	228	ASP
3	n	237	VAL
3	n	238	ILE
3	n	271	ASN
3	n	279	THR
3	n	366	ASN
3	n	391	ILE
3	o	114	ASP
3	o	147	ARG
3	o	245	THR
3	o	272	THR
3	o	279	THR
3	o	301	THR
3	o	324	LEU
3	o	326	ILE
3	o	395	LEU
4	q	166	PHE
4	q	199	VAL
4	q	238	VAL
4	q	322	THR
4	q	366	PHE
4	q	371	ASN
4	q	382	LEU
4	q	411	LEU
4	q	536	LEU
4	q	557	LEU
4	q	577	GLN
4	q	607	ASN
4	q	651	ILE
4	q	767	THR

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Mol	Chain	Res	Type
4	q	800	TYR
4	q	811	LEU
4	q	817	TRP
4	q	826	TYR
4	q	871	PHE
4	q	880	LEU
4	r	79	LYS
4	r	88	TYR
4	r	94	THR
4	r	105	LEU
4	r	114	GLU
4	r	129	ARG
4	r	135	ILE
4	r	166	PHE
4	r	192	ASN
4	r	281	ASP
4	r	298	TYR
4	r	382	LEU
4	r	387	LEU
4	r	395	ASP
4	r	411	LEU
4	r	466	PHE
4	r	476	ASN
4	r	480	PHE
4	r	483	VAL
4	r	485	ILE
4	r	518	PHE
4	r	523	VAL
4	r	578	LEU
4	r	590	ASN
4	r	619	ASN
4	r	629	ASN
4	r	634	TYR
4	r	656	VAL
4	r	690	ASP
4	r	721	VAL
4	r	749	ASN
4	r	803	ASN
4	r	880	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	632	ASN
2	E	308	GLN
2	F	182	ASN
2	I	305	GLN
2	J	262	GLN
2	J	288	ASN
2	K	308	GLN
3	f	351	GLN
3	g	239	ASN
3	g	310	ASN
3	h	316	HIS
3	j	26	ASN
3	l	170	GLN
3	m	112	GLN
3	n	381	ASN
3	o	345	ASN
4	r	192	ASN
4	r	246	HIS
4	r	609	ASN
4	r	746	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

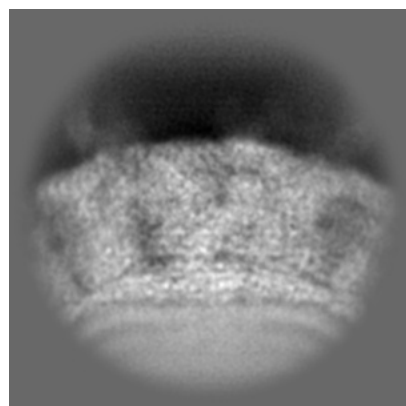
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16772. These allow visual inspection of the internal detail of the map and identification of artifacts.

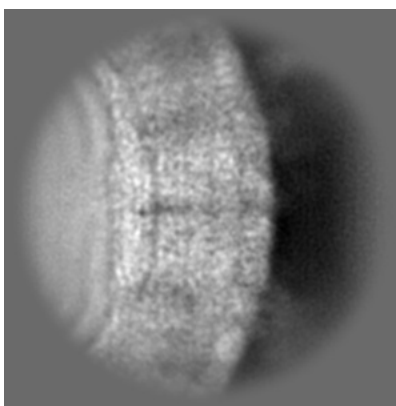
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

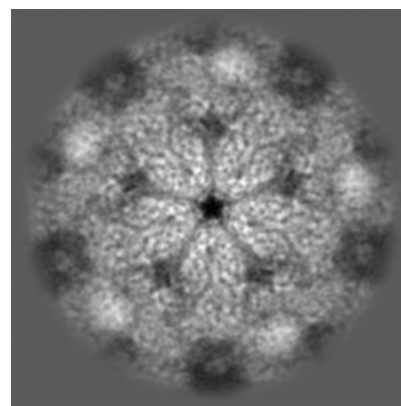
6.1.1 Primary map



X

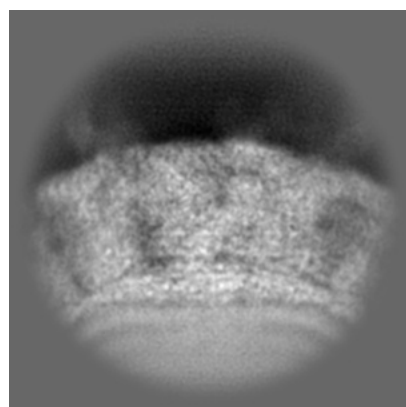


Y

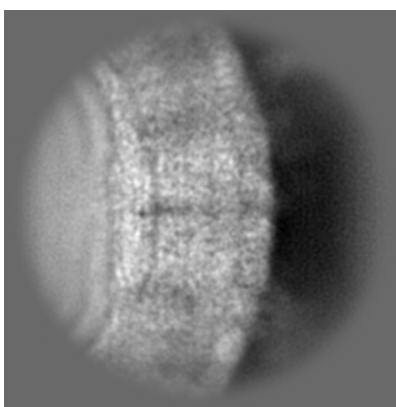


Z

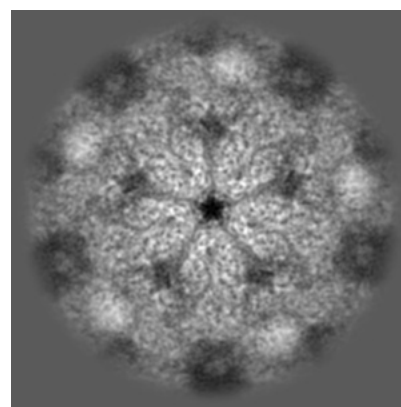
6.1.2 Raw map



X



Y

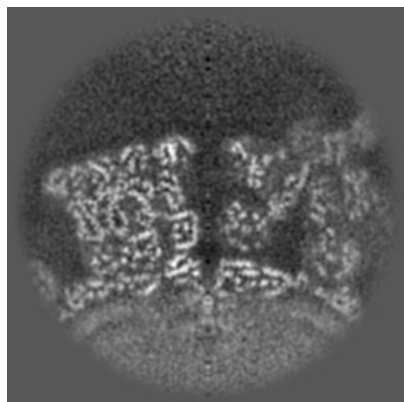


Z

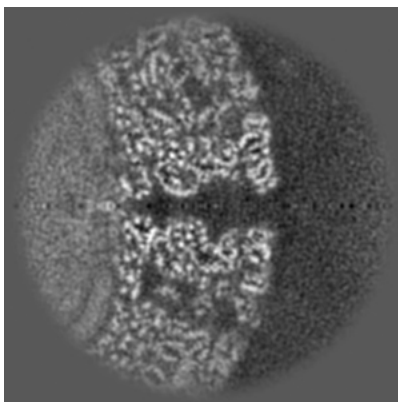
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

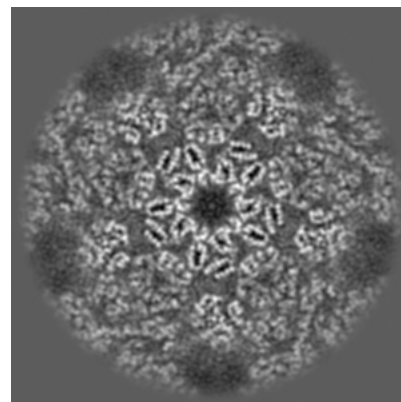
6.2.1 Primary map



X Index: 105

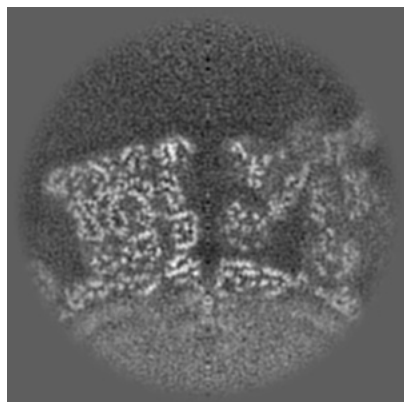


Y Index: 105

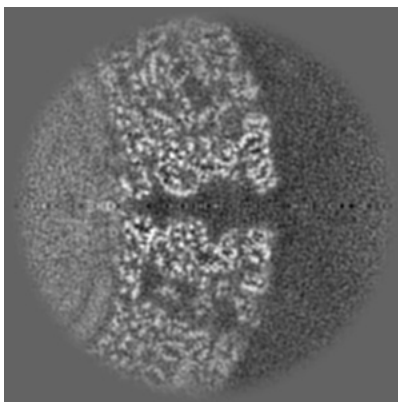


Z Index: 105

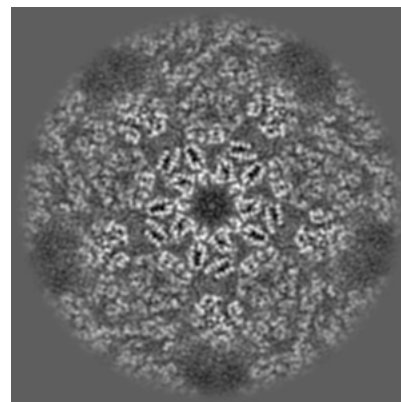
6.2.2 Raw map



X Index: 105



Y Index: 105

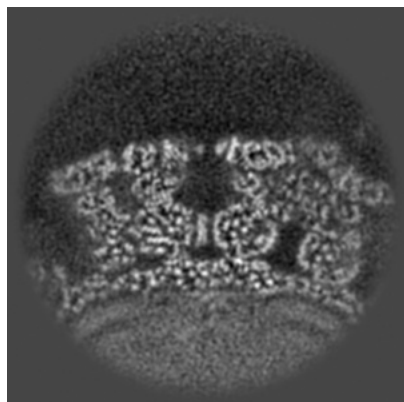


Z Index: 105

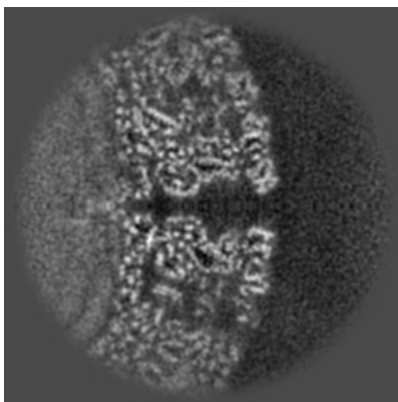
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

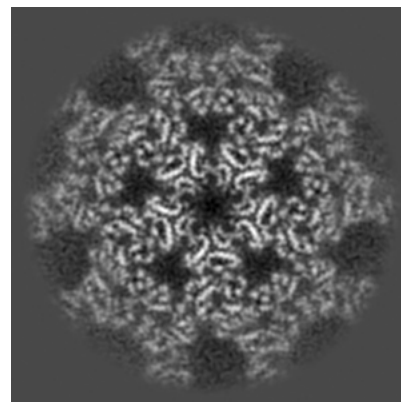
6.3.1 Primary map



X Index: 99

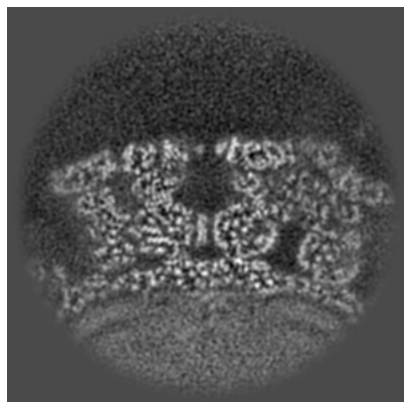


Y Index: 104

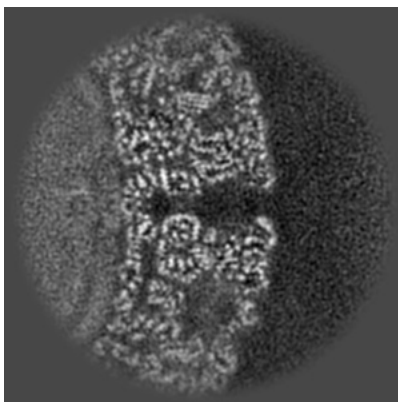


Z Index: 82

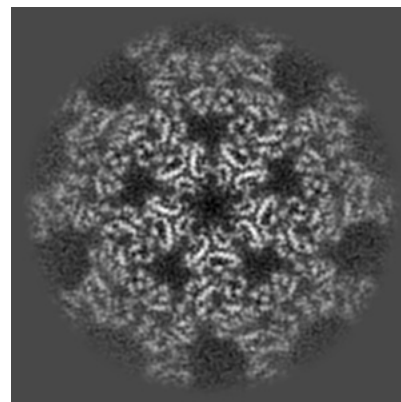
6.3.2 Raw map



X Index: 99



Y Index: 101

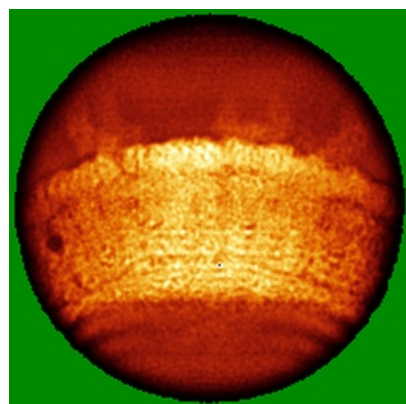


Z Index: 82

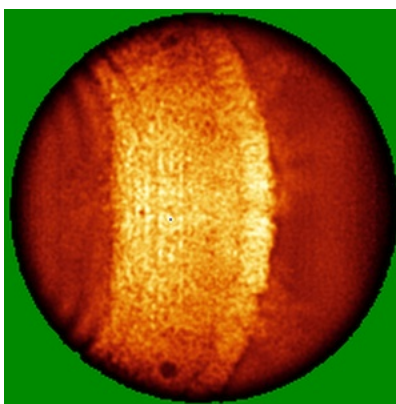
The images above show the largest variance slices of the map in three orthogonal directions.

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

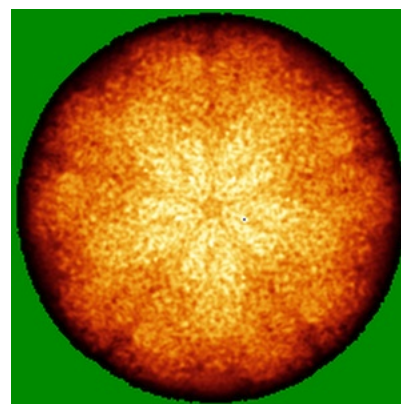
6.4.1 Primary map



X

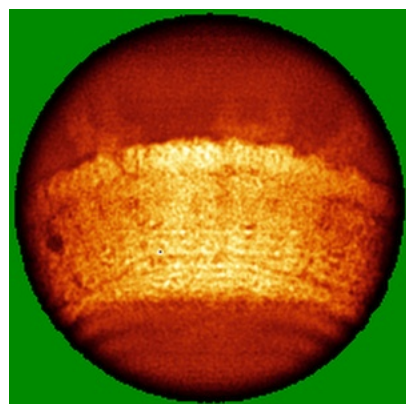


Y

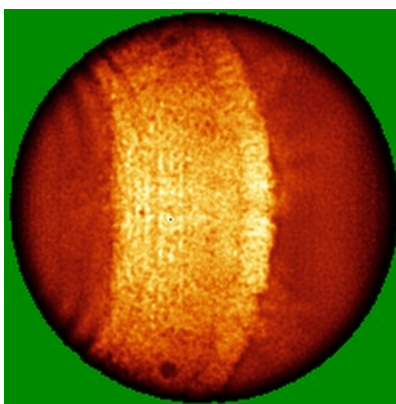


Z

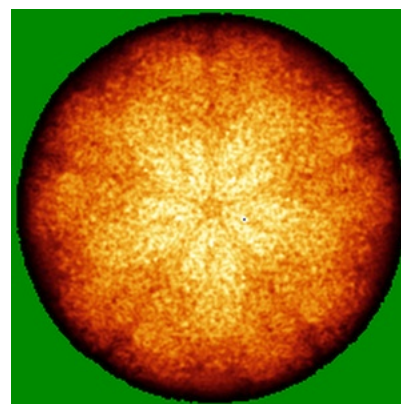
6.4.2 Raw map



X



Y

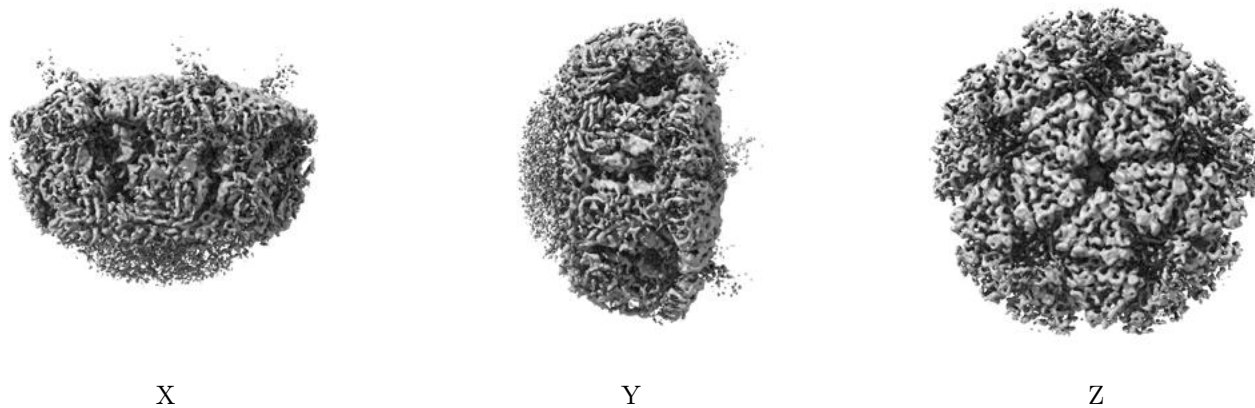


Z

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.

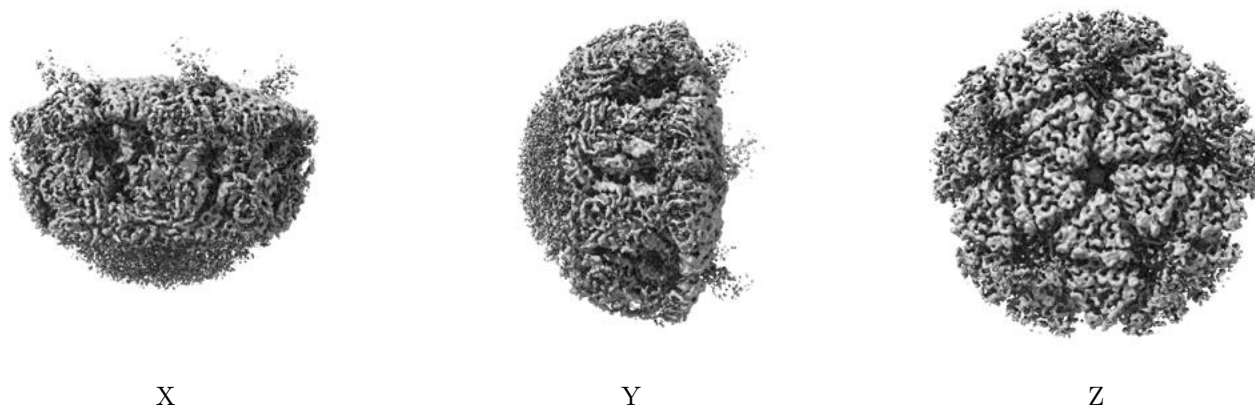
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

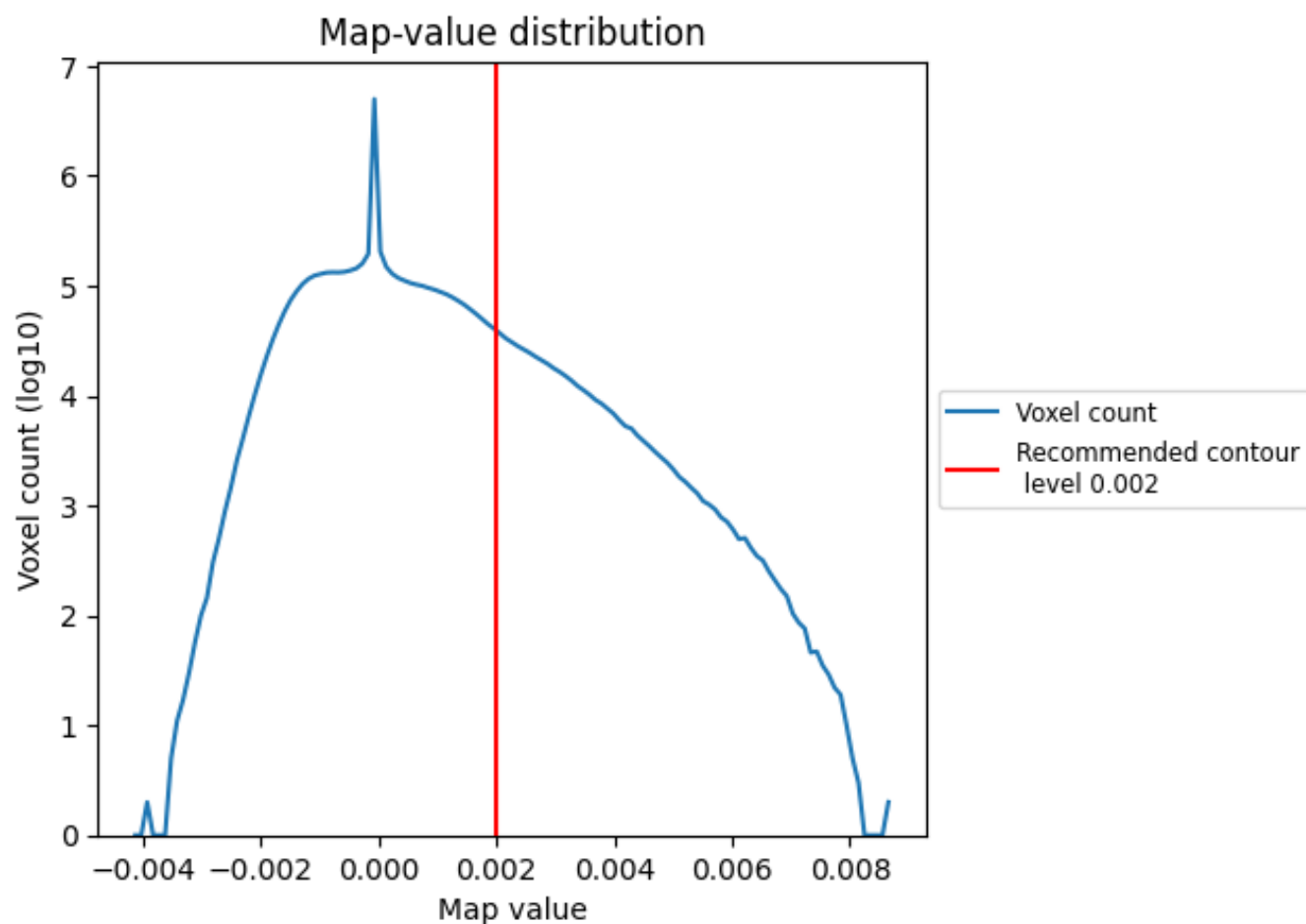
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

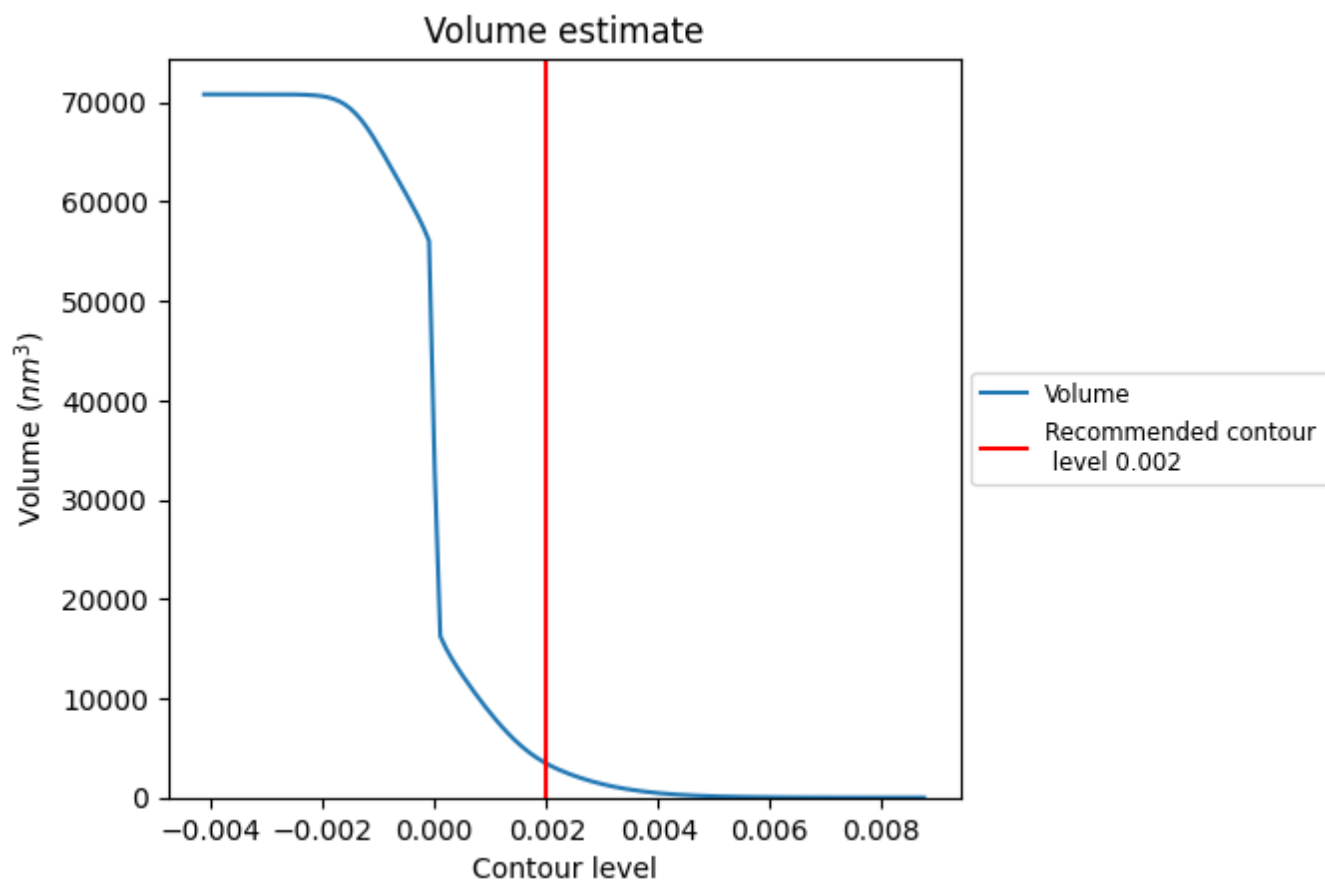
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

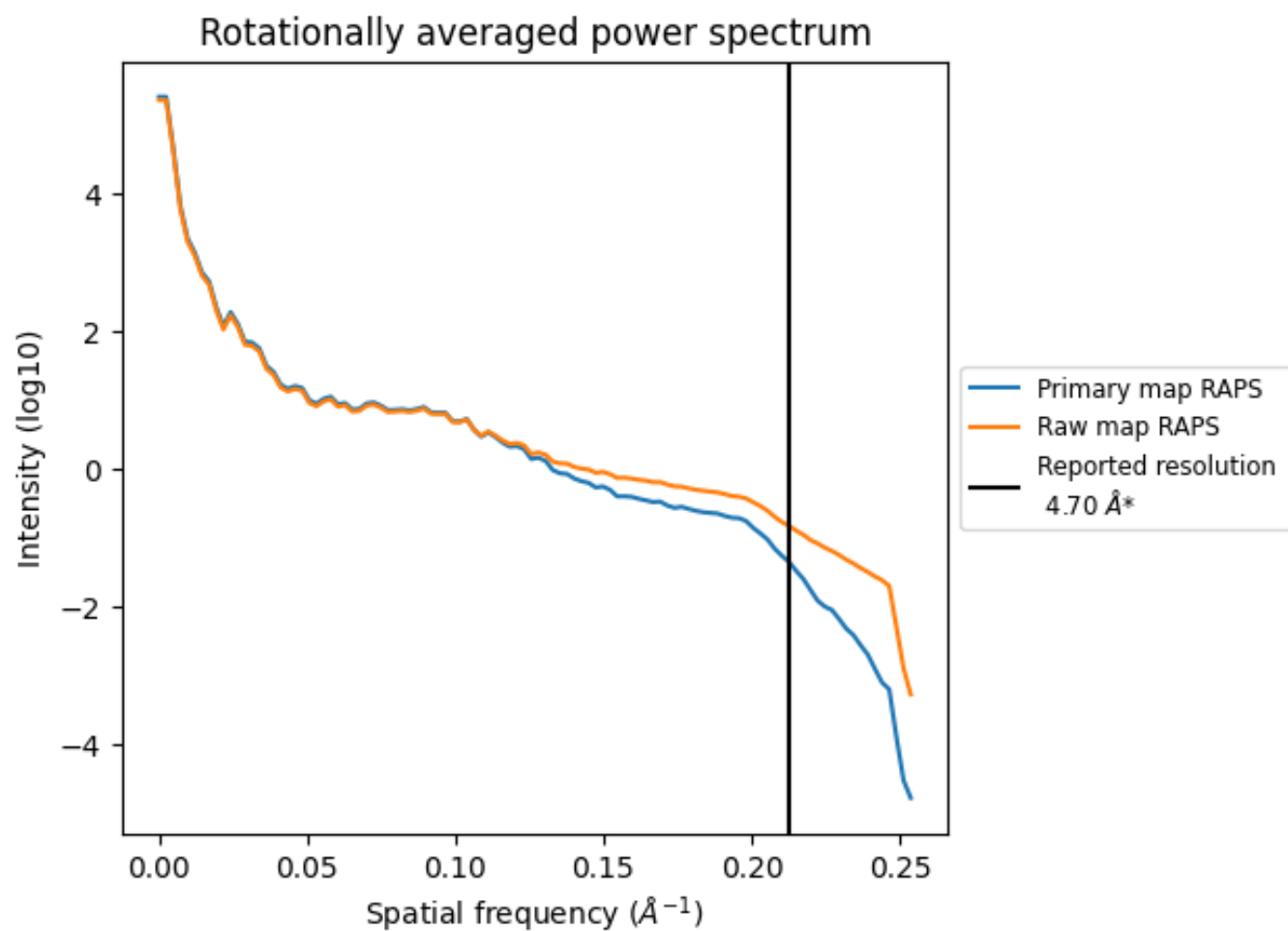
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3431 nm³; this corresponds to an approximate mass of 3099 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

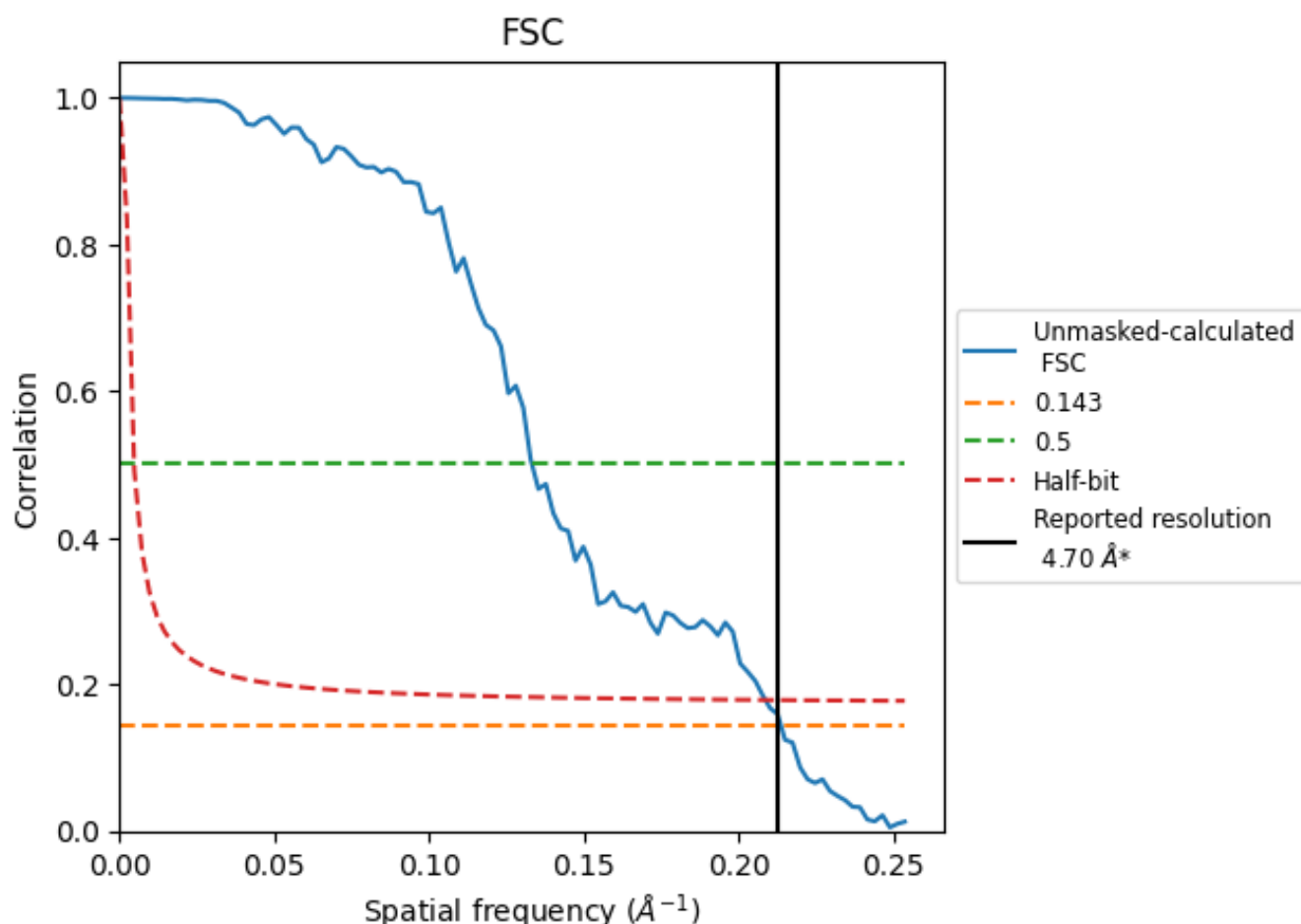


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.213 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	7.50	4.79

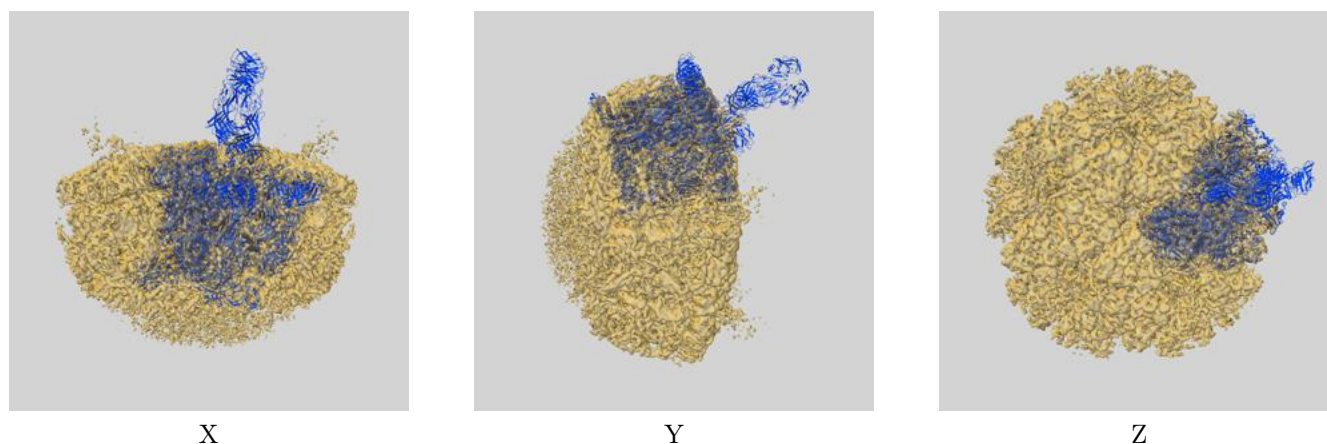
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

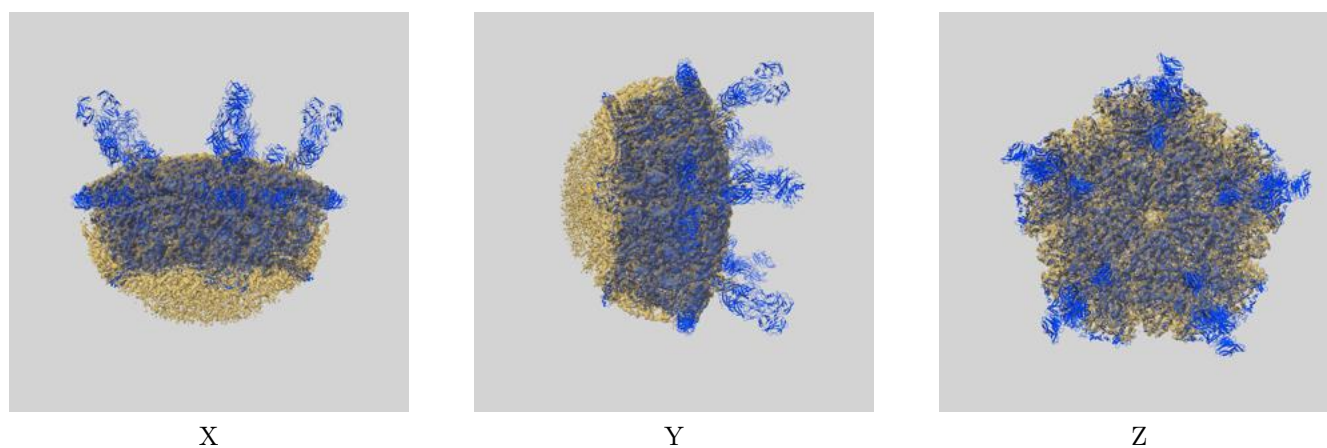
This section contains information regarding the fit between EMDB map EMD-16772 and PDB model 8CO6. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

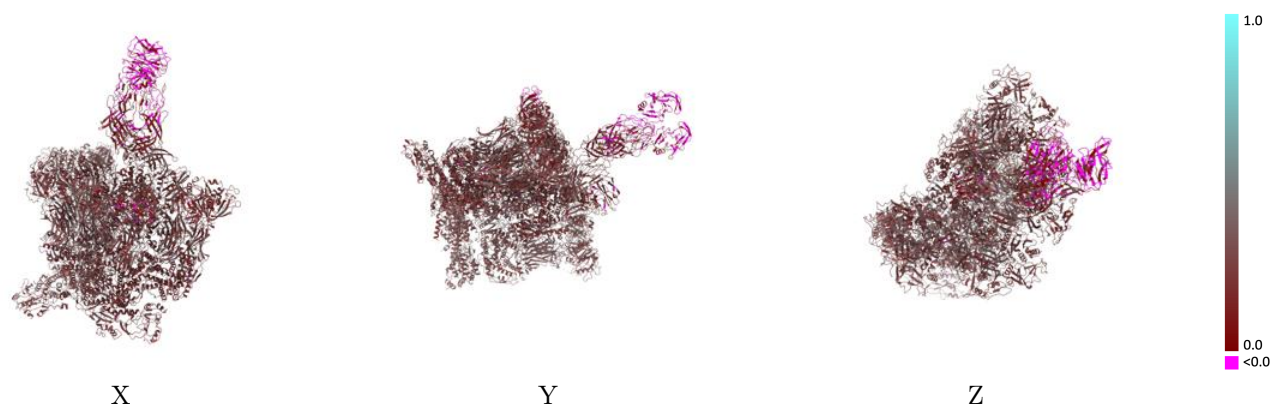


9.1.2 Map-model assembly overlay [i](#)



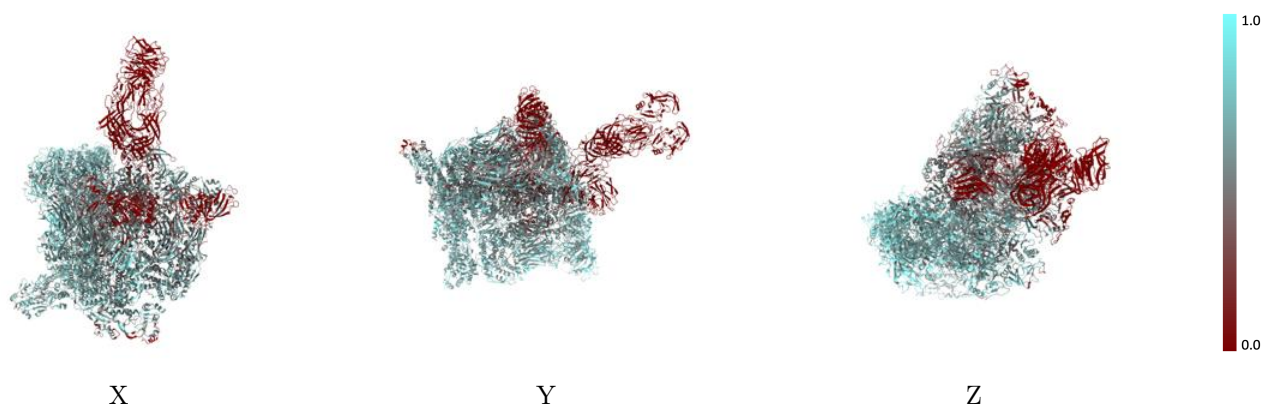
The images above show the 3D surface view of the map at the recommended contour level 0.002 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



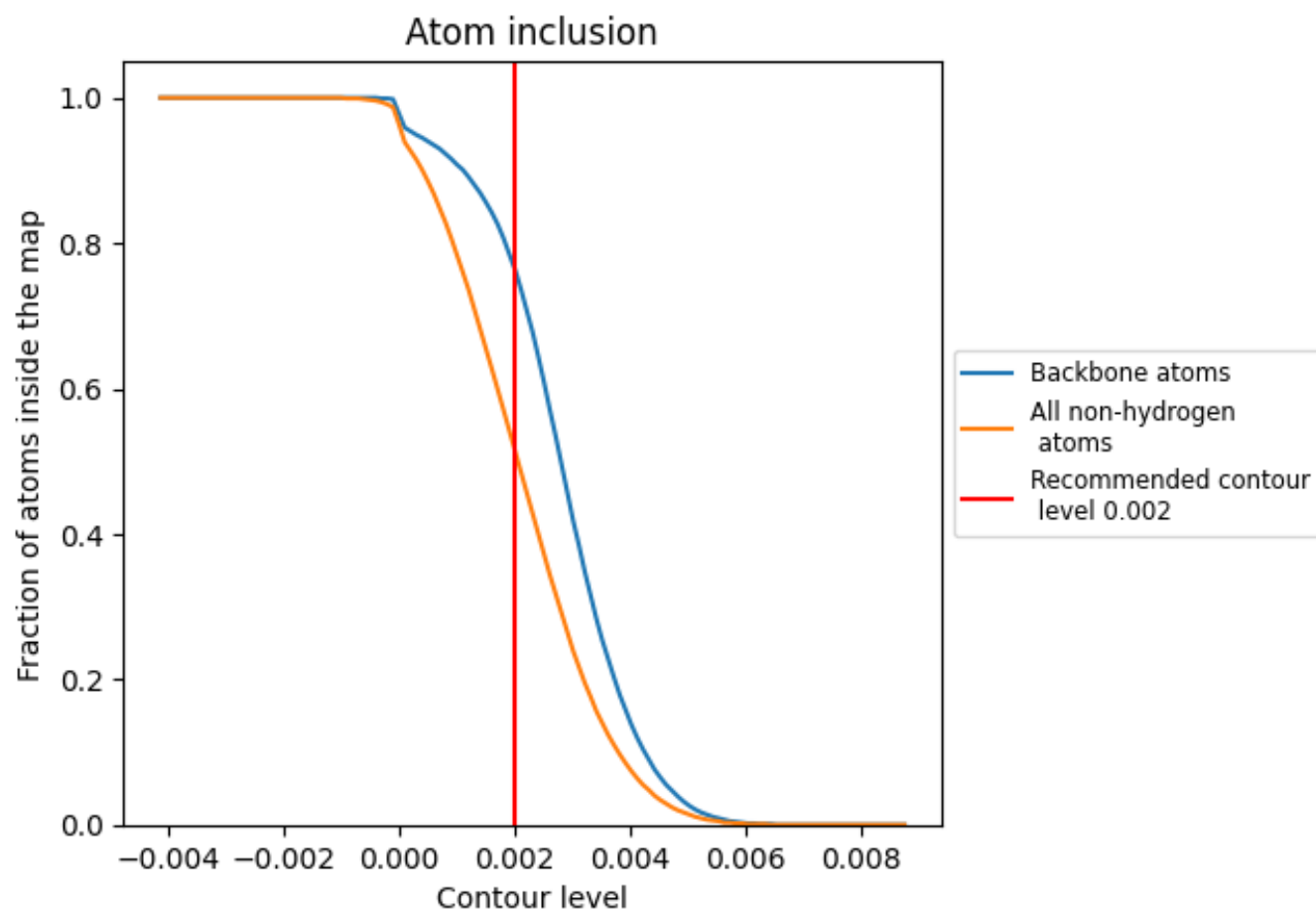
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.5180	 0.2680
A	 0.1630	 0.1590
B	 0.1490	 0.1660
C	 0.2990	 0.2630
D	 0.5050	 0.2760
E	 0.1650	 0.2560
F	 0.3620	 0.2610
G	 0.3430	 0.2750
H	 0.1450	 0.2170
I	 0.4750	 0.2870
J	 0.6030	 0.2960
K	 0.6240	 0.2860
L	 0.6770	 0.2890
M	 0.6990	 0.2920
N	 0.7470	 0.2970
O	 0.7440	 0.3030
d	 0.5590	 0.2900
e	 0.5760	 0.2830
f	 0.5430	 0.2850
g	 0.5770	 0.2890
h	 0.5630	 0.2840
i	 0.5240	 0.2870
j	 0.6230	 0.2870
k	 0.6650	 0.2890
l	 0.6620	 0.2900
m	 0.7060	 0.2970
n	 0.7040	 0.2990
o	 0.7110	 0.3000
q	 0.6830	 0.2830
r	 0.6270	 0.2790

