wwPDB EM Validation Summary Report

May 2, 2023 – 02:11 pm BST

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 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 (i) symbol.

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

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

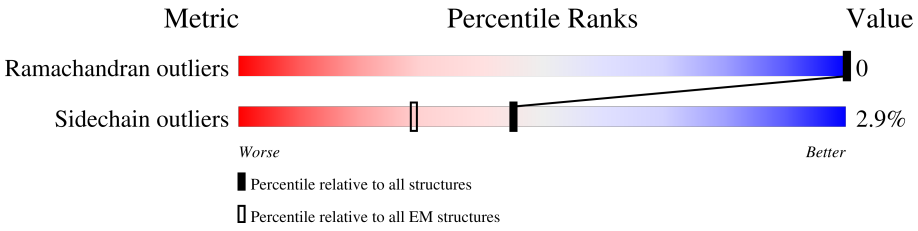
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 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	154571	4023
Sidechain outliers	154315	3826

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	A	776	73% 90% · 6%
1	B	776	77% 94% · ·
1	C	776	52% 87% · 11%
2	D	326	25% 79% · 20%
2	E	326	62% 73% · 25%
2	F	326	43% 80% · 18%
2	G	326	45% 81% · 18%
2	H	326	63% 72% · 26%
2	I	326	30% 79% · 19%

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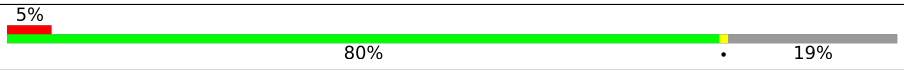
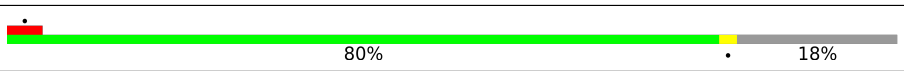
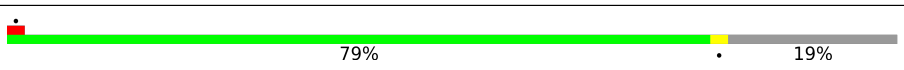
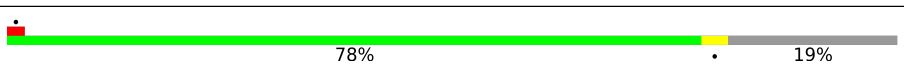
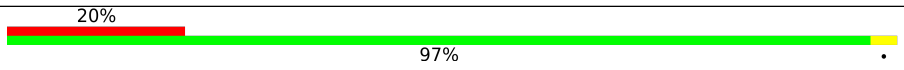
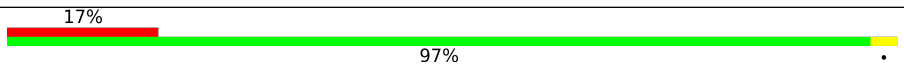
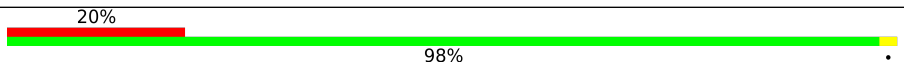
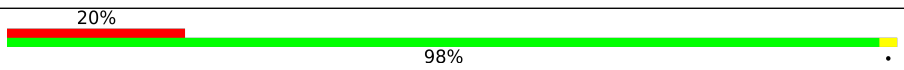
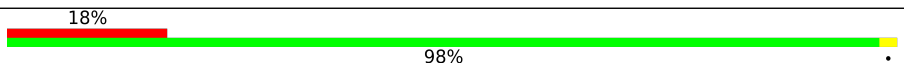
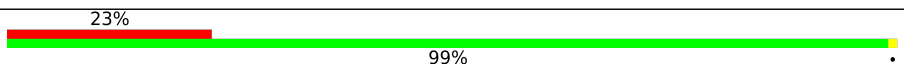
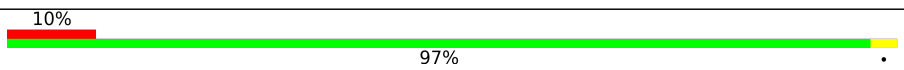
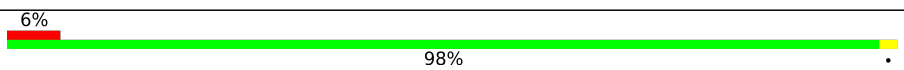
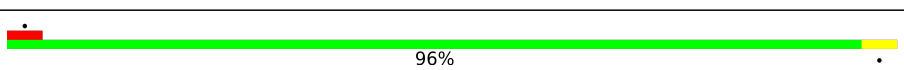
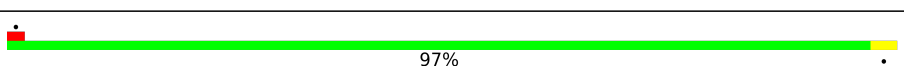
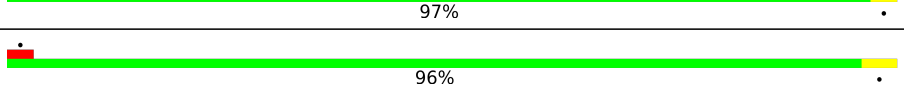
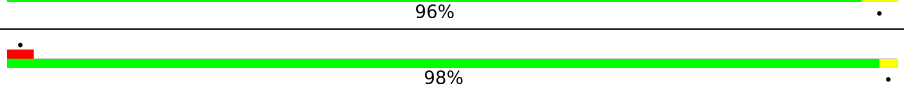
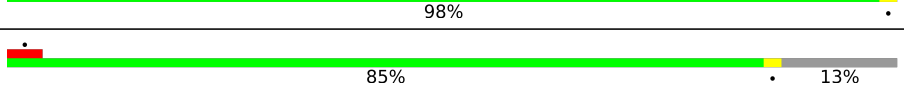
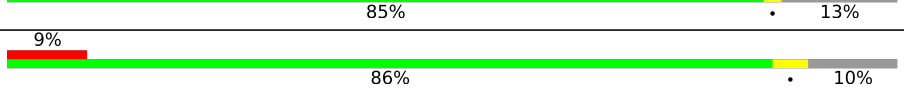
Mol	Chain	Length	Quality of chain
2	J	326	
2	K	326	
2	L	326	
2	M	326	
2	N	326	
2	O	326	
3	d	397	
3	e	397	
3	f	397	
3	g	397	
3	h	397	
3	i	397	
3	j	397	
3	k	397	
3	l	397	
3	m	397	
3	n	397	
3	o	397	
4	q	882	
4	r	882	

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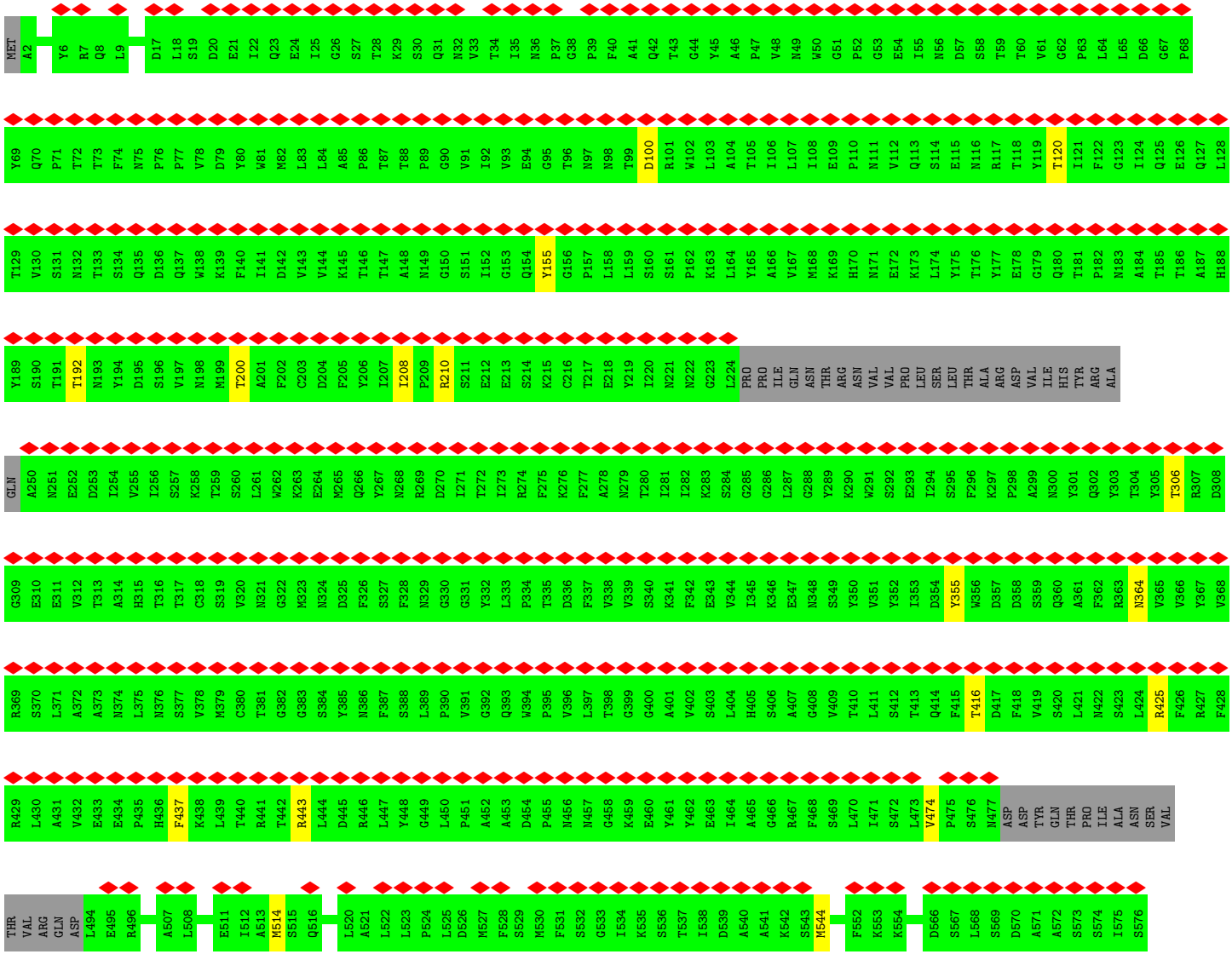
Chain	Residue	Modelled	Actual	Comment	Reference
r	766	VAL	ILE	conflict	UNP A2T3R1
r	777	ILE	LYS	conflict	UNP A2T3R1
r	818	VAL	ILE	conflict	UNP A2T3R1
r	820	ILE	THR	conflict	UNP A2T3R1
r	831	VAL	GLN	conflict	UNP A2T3R1
r	837	ASN	ALA	conflict	UNP A2T3R1

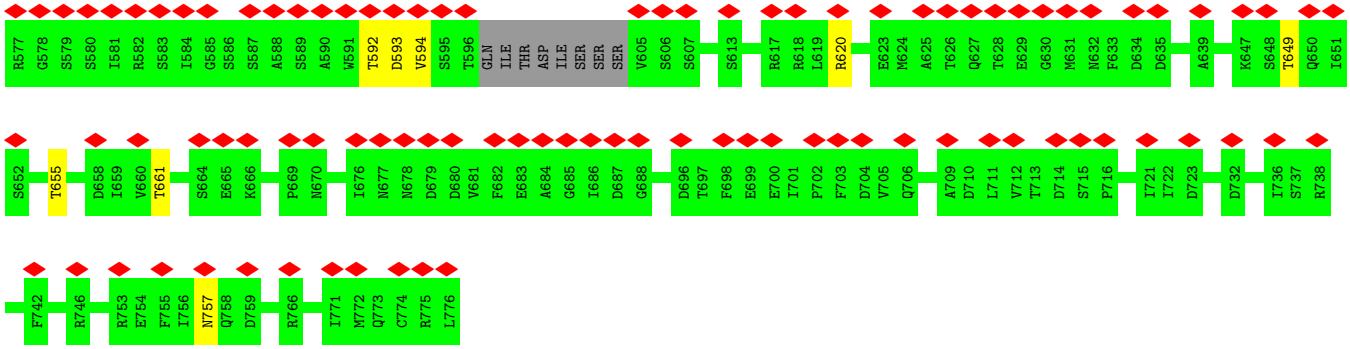
3 Residue-property plots (i)

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

- Molecule 1: Outer capsid protein VP4

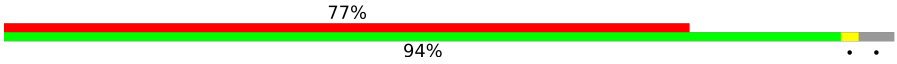
Chain A:

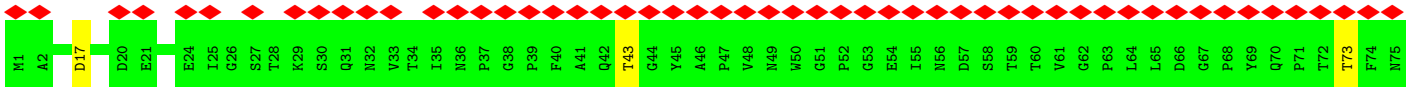


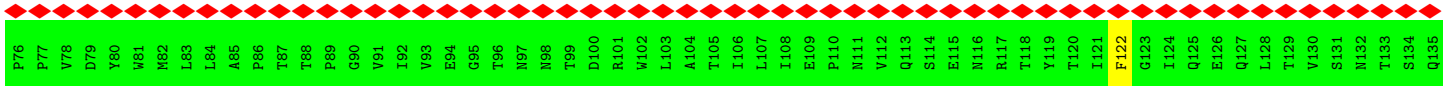


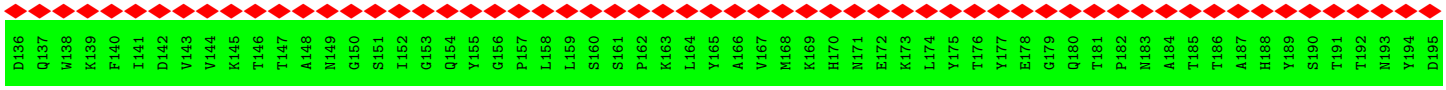
• Molecule 1: Outer capsid protein VP4

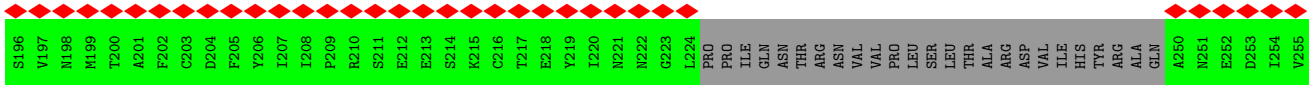
Chain B:

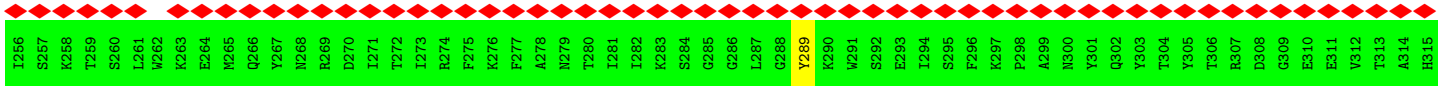


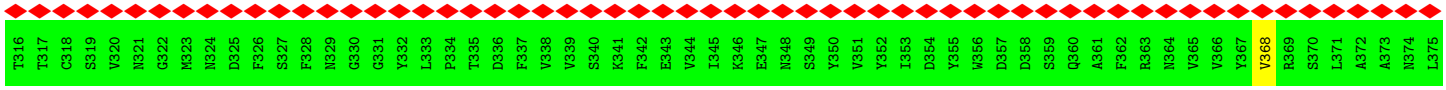


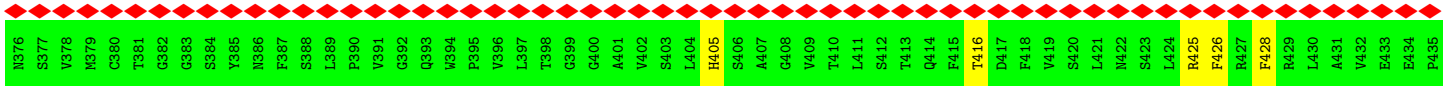


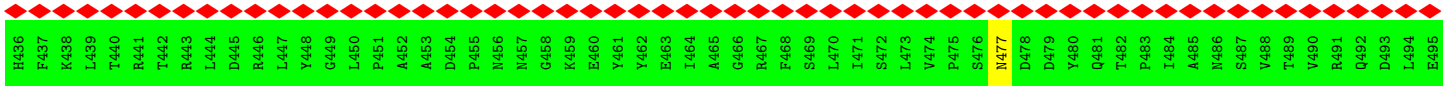


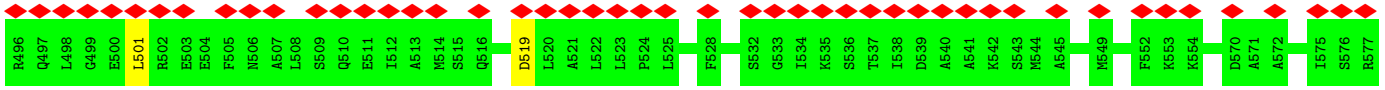


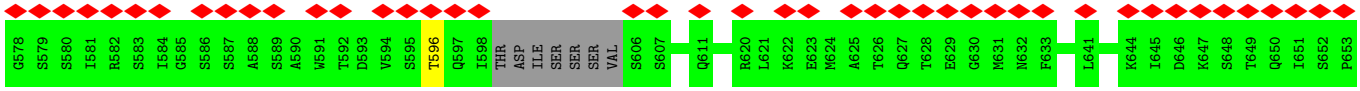


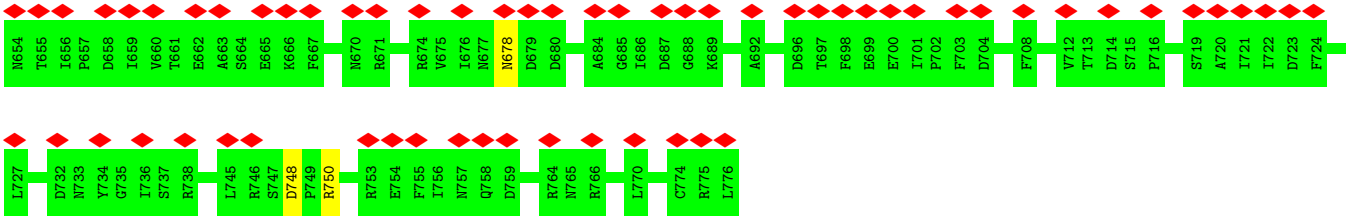




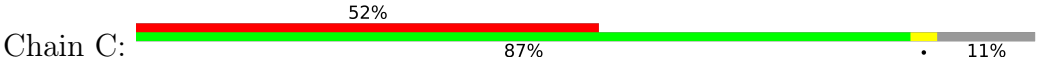


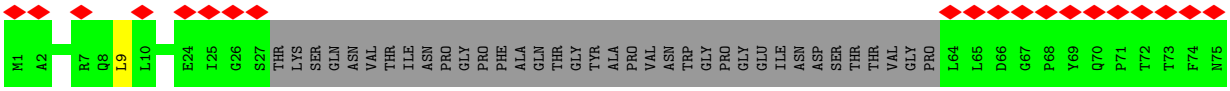


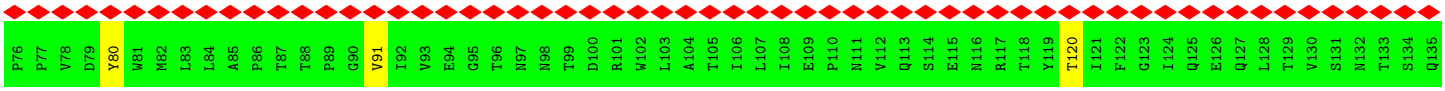


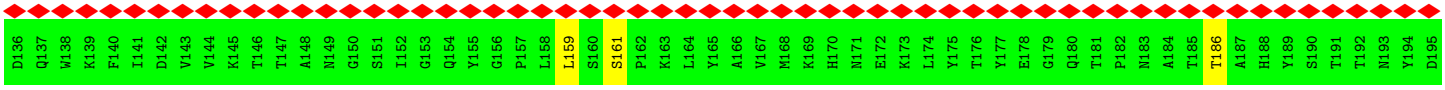


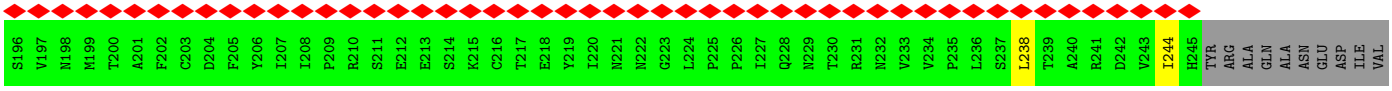
• Molecule 1: Outer capsid protein VP4

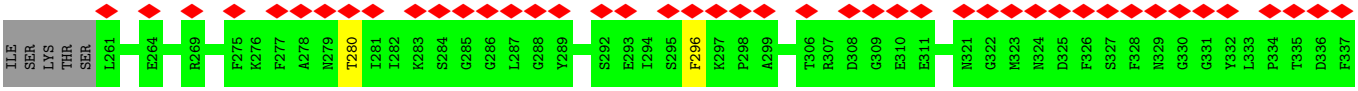


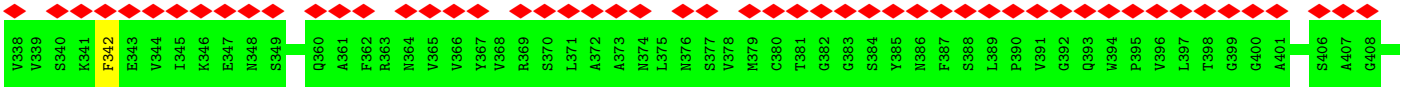


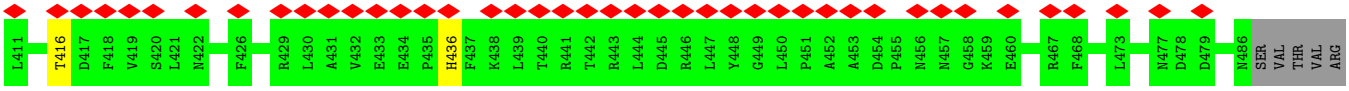


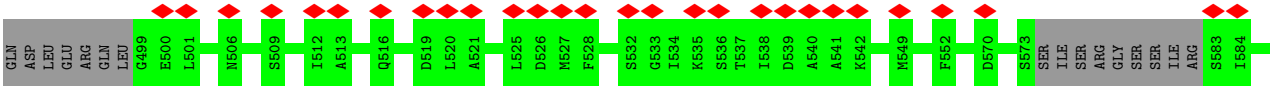


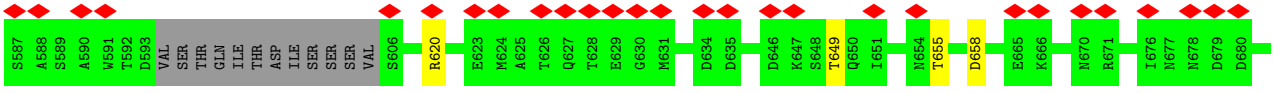


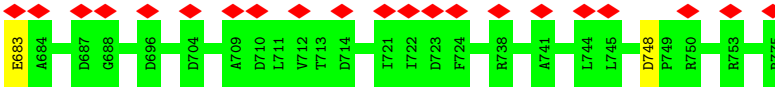






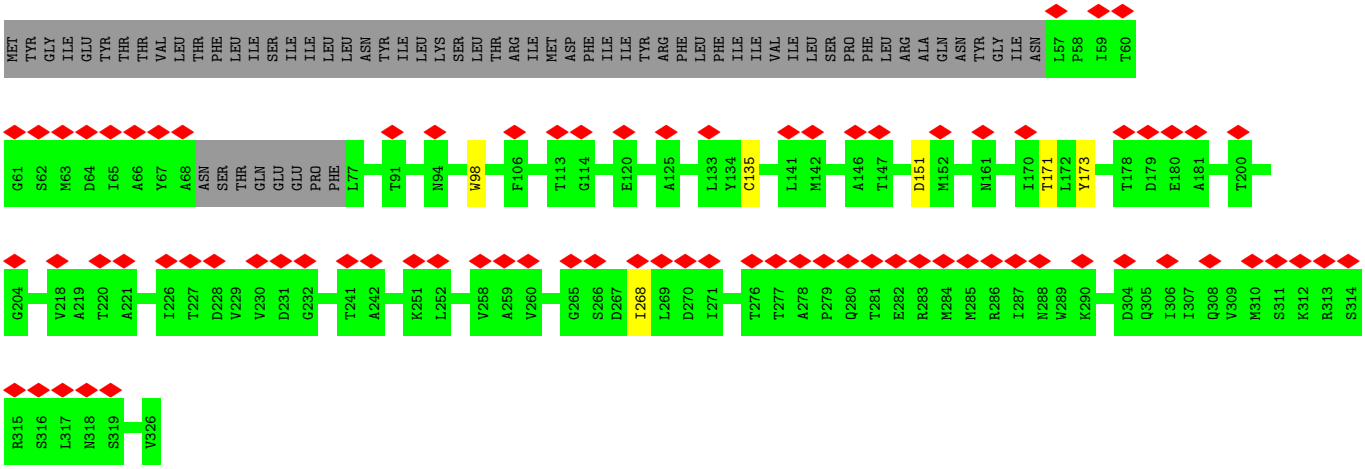






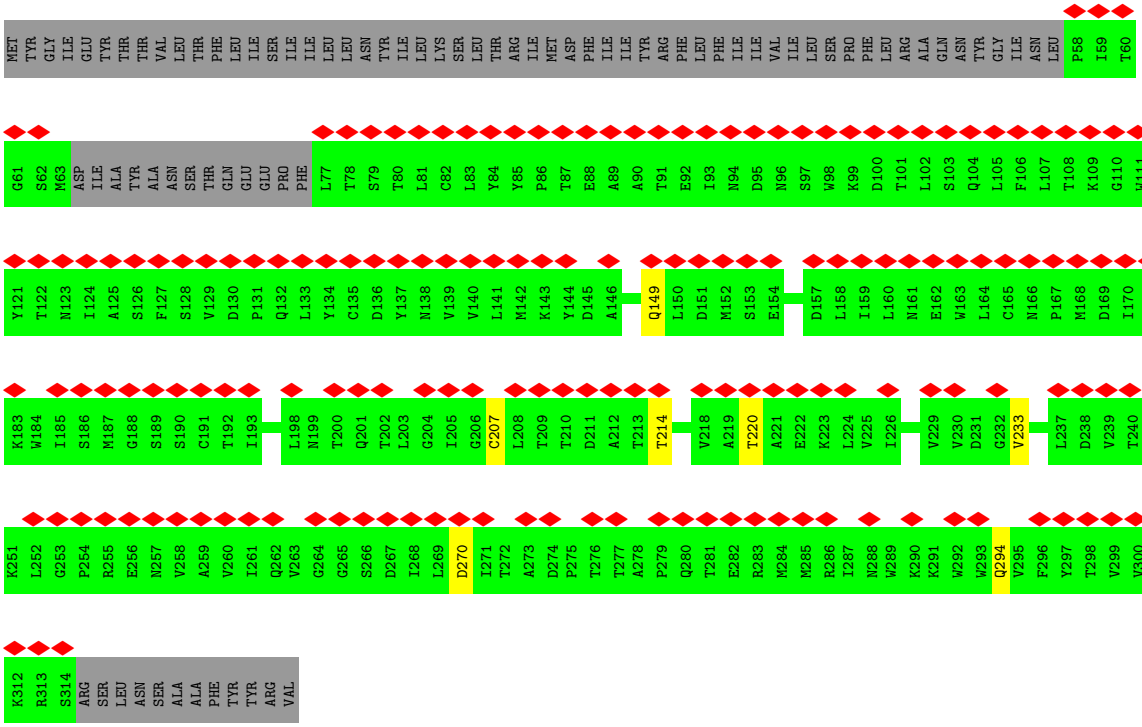
• Molecule 2: Outer capsid glycoprotein VP7

Chain D:



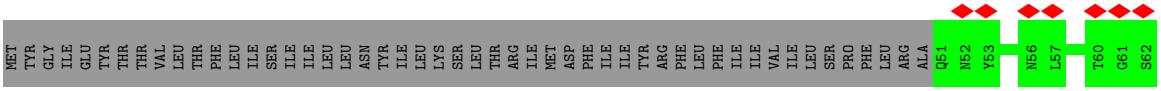
• Molecule 2: Outer capsid glycoprotein VP7

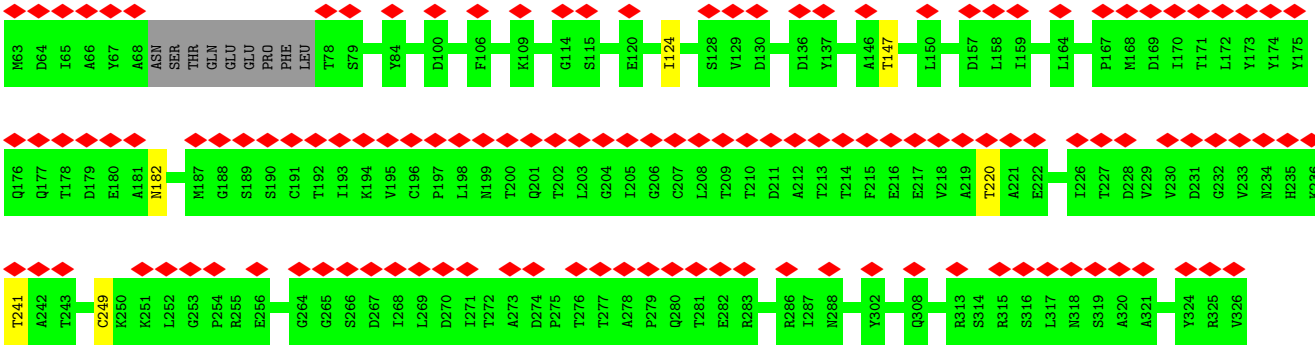
Chain E:



• Molecule 2: Outer capsid glycoprotein VP7

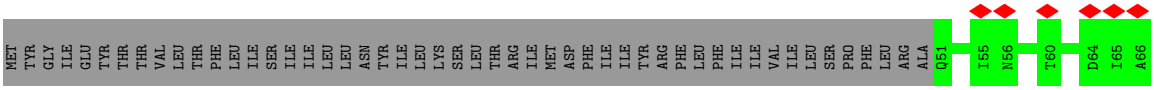
Chain F:

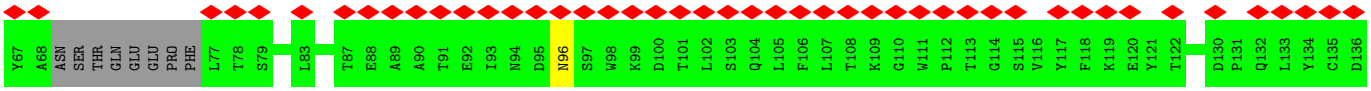


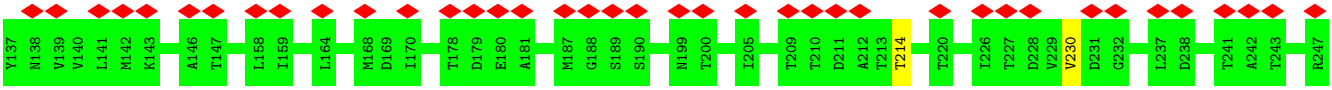


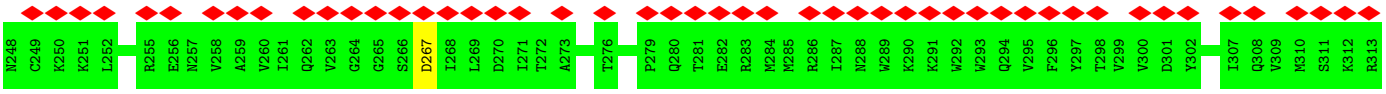
• Molecule 2: Outer capsid glycoprotein VP7

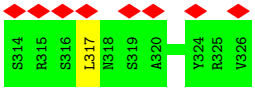
Chain G:





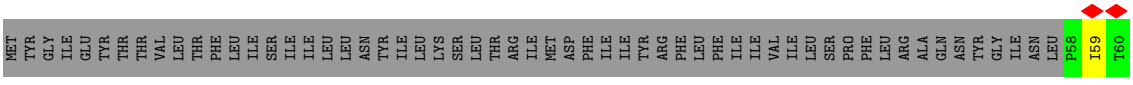


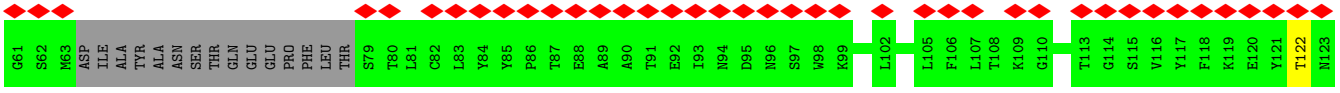


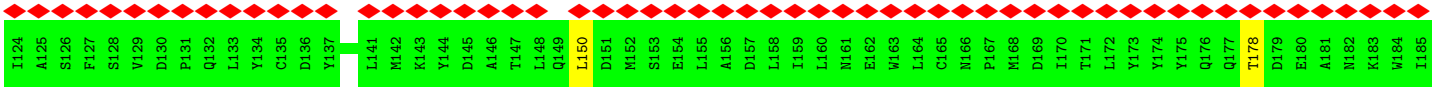


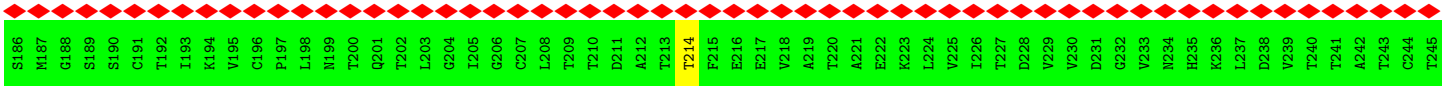
• Molecule 2: Outer capsid glycoprotein VP7

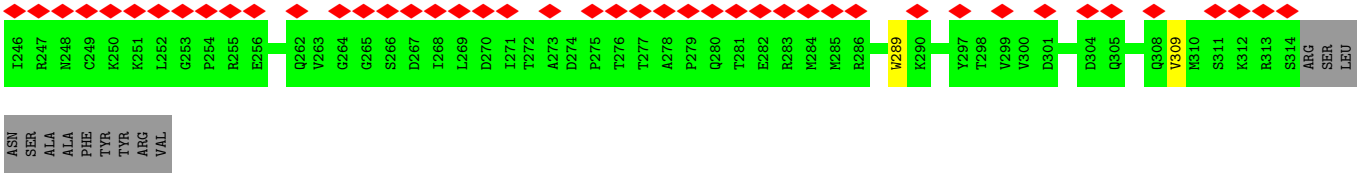
Chain H:





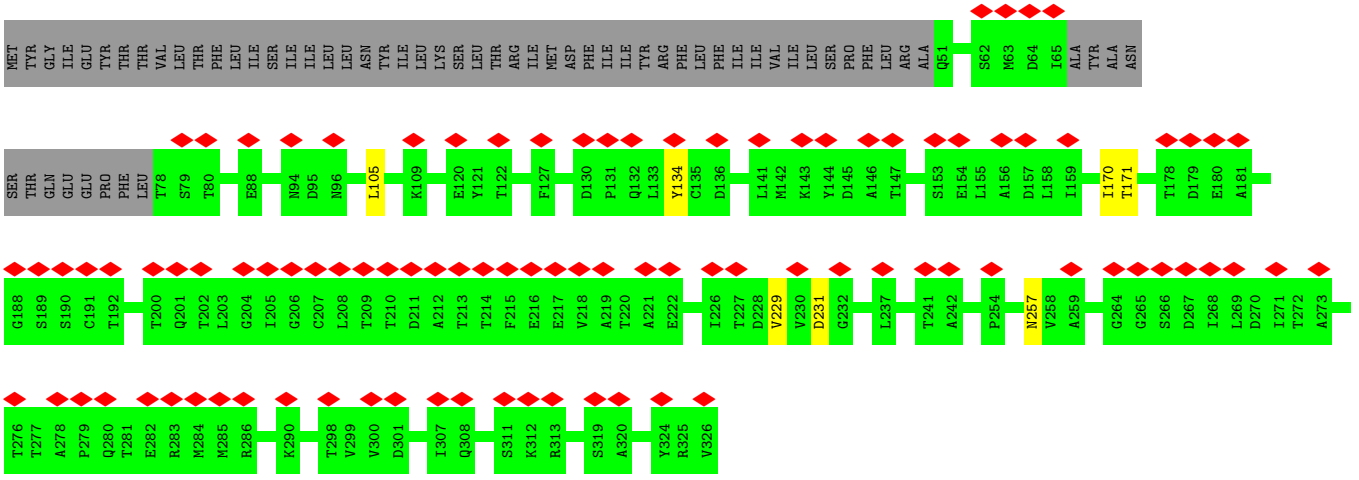






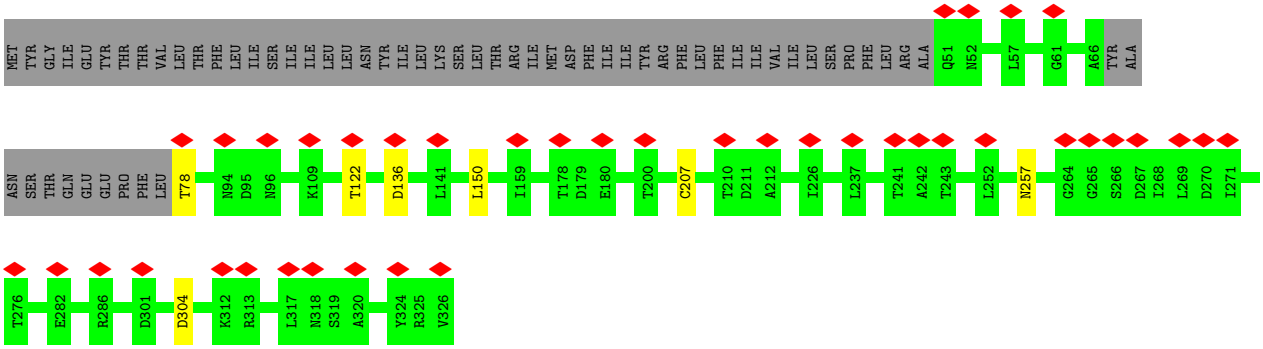
• Molecule 2: Outer capsid glycoprotein VP7

Chain I:



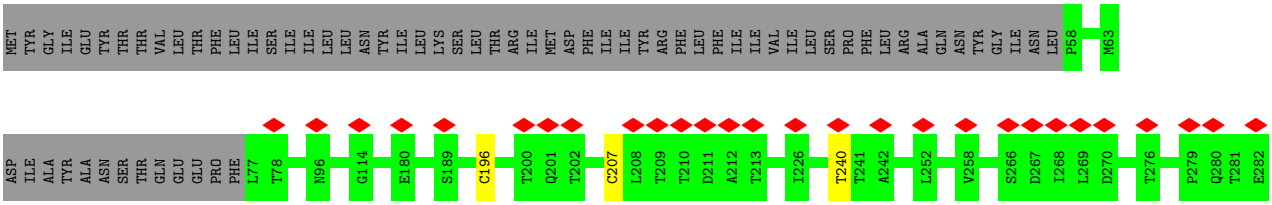
• Molecule 2: Outer capsid glycoprotein VP7

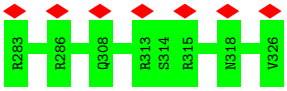
Chain J:



• Molecule 2: Outer capsid glycoprotein VP7

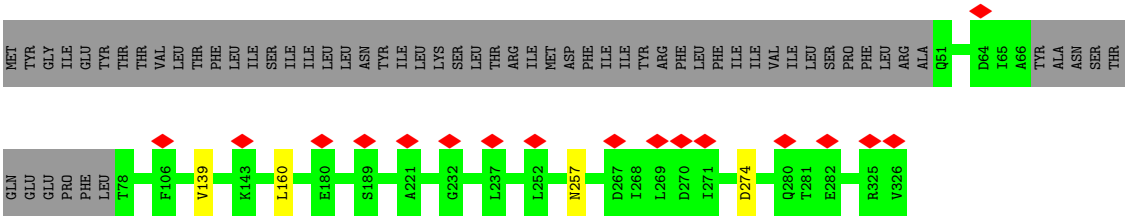
Chain K:





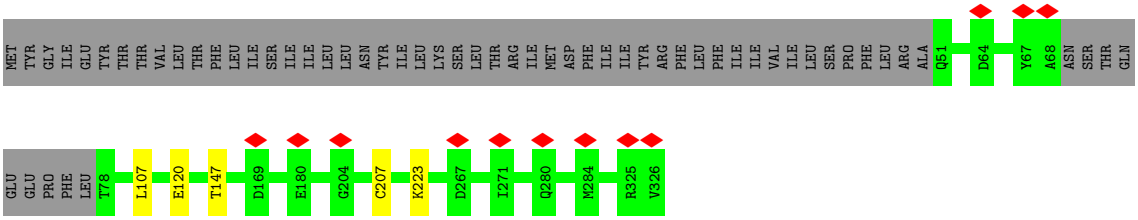
• Molecule 2: Outer capsid glycoprotein VP7

Chain L:



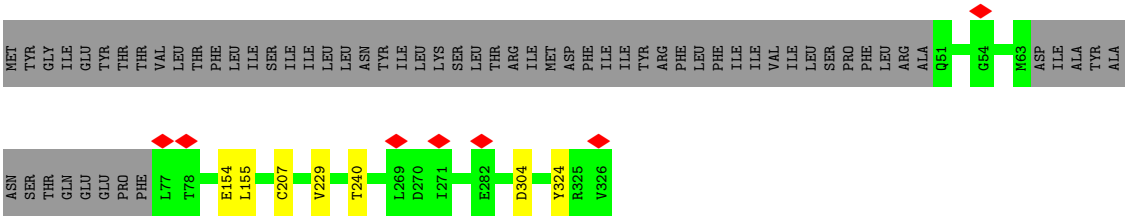
• Molecule 2: Outer capsid glycoprotein VP7

Chain M:



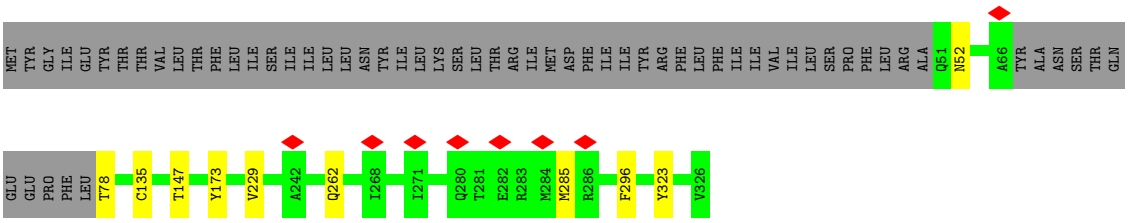
• Molecule 2: Outer capsid glycoprotein VP7

Chain N:



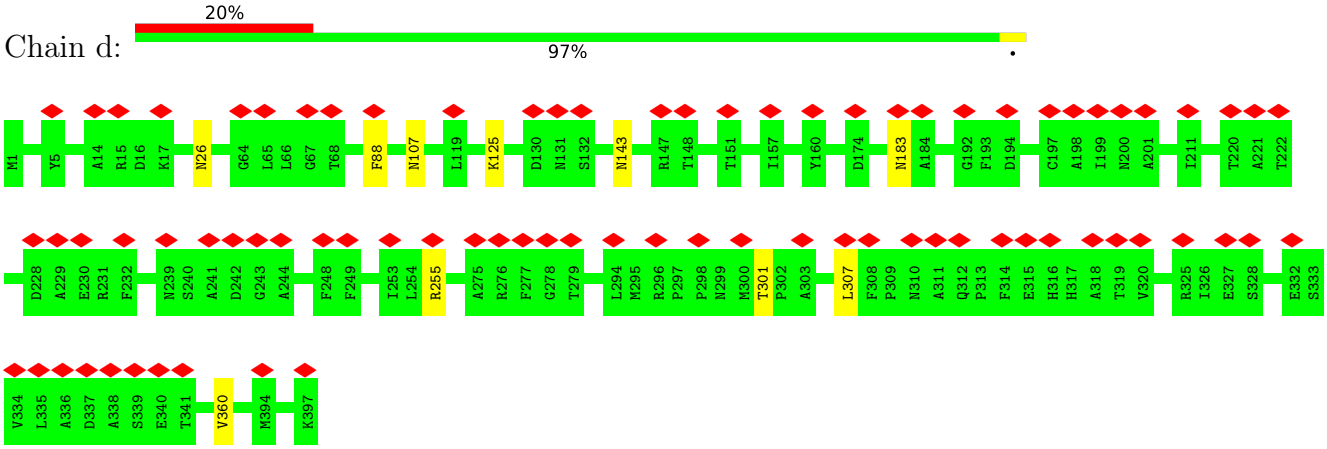
• Molecule 2: Outer capsid glycoprotein VP7

Chain O:



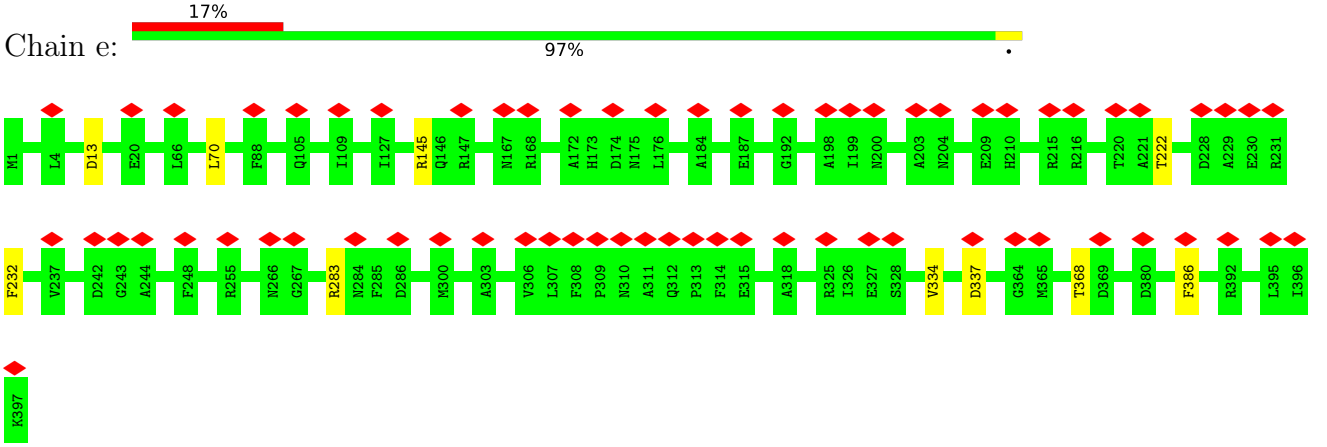
• Molecule 3: Intermediate capsid protein VP6

Chain d:



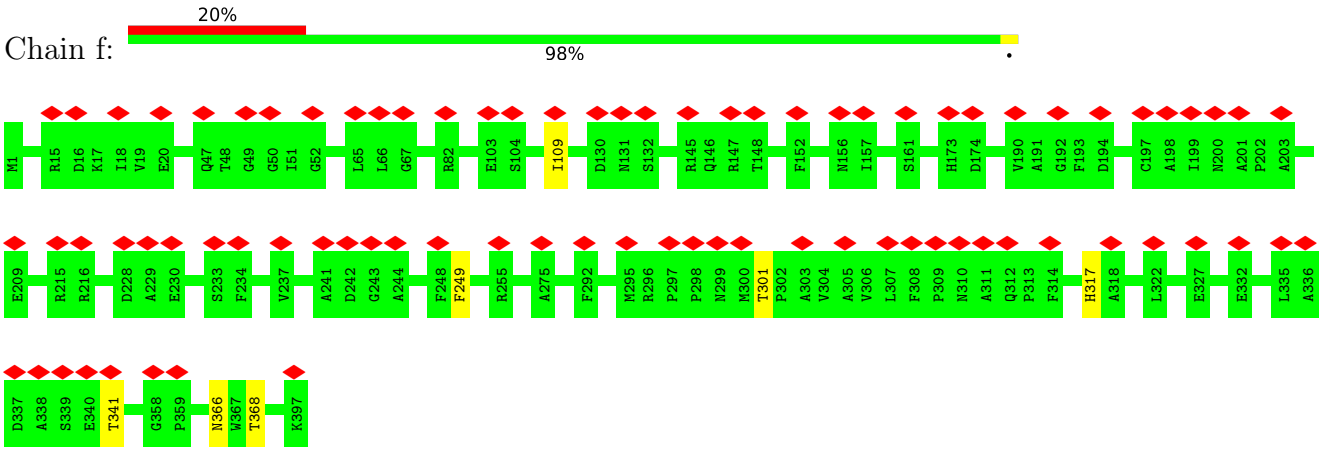
• Molecule 3: Intermediate capsid protein VP6

Chain e:



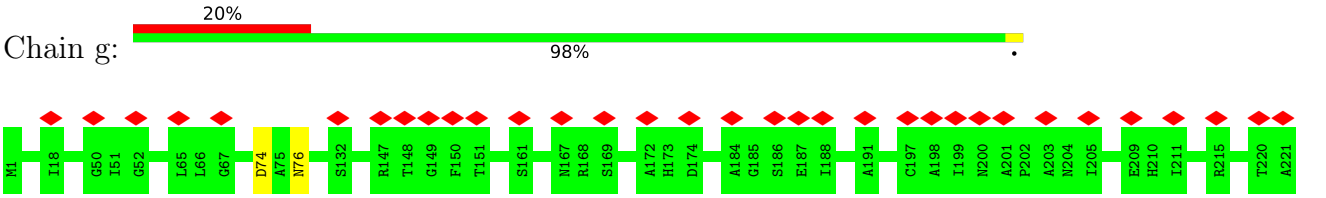
• Molecule 3: Intermediate capsid protein VP6

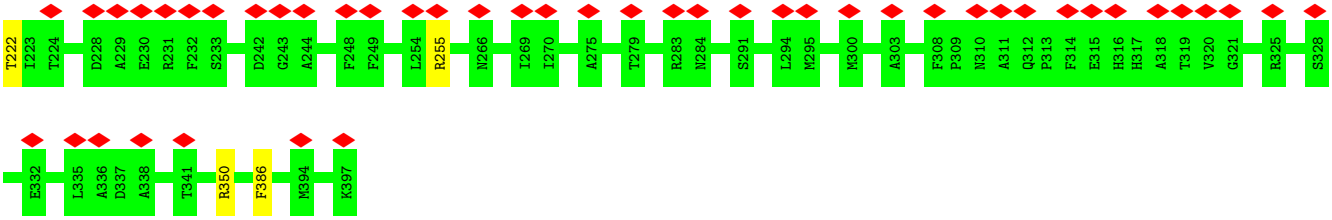
Chain f:



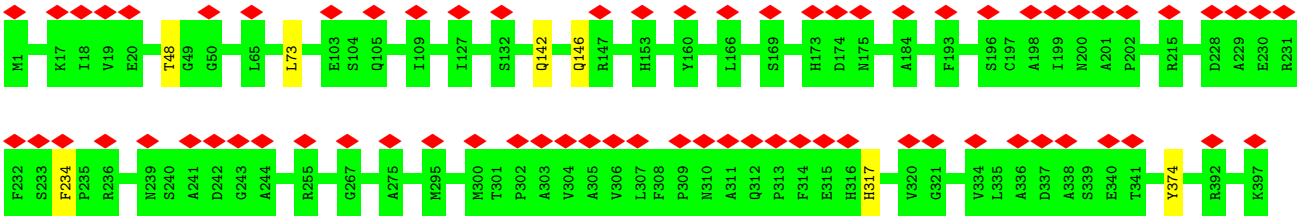
• Molecule 3: Intermediate capsid protein VP6

Chain g:

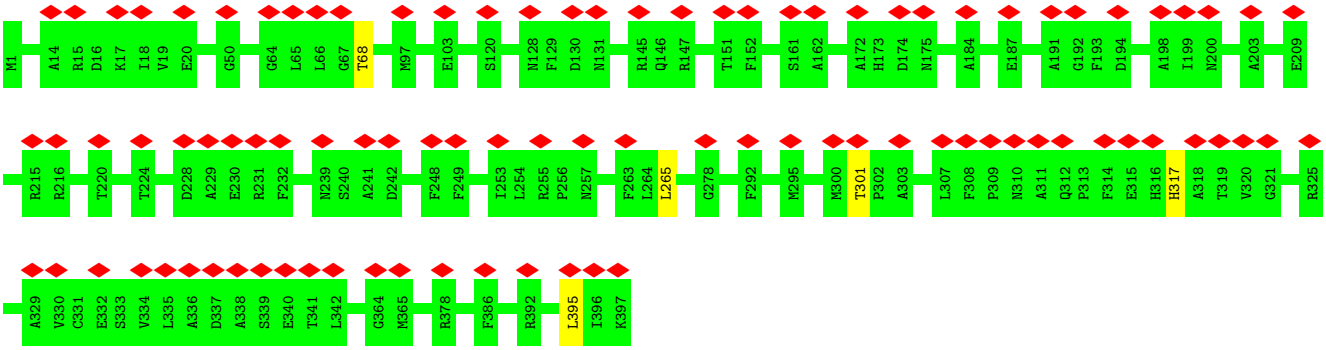




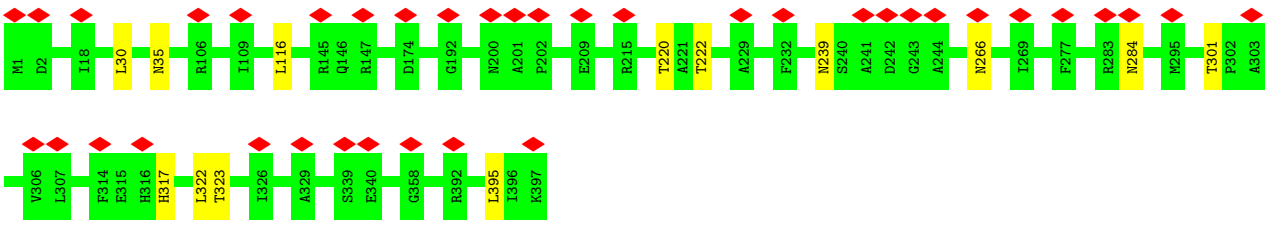
• Molecule 3: Intermediate capsid protein VP6



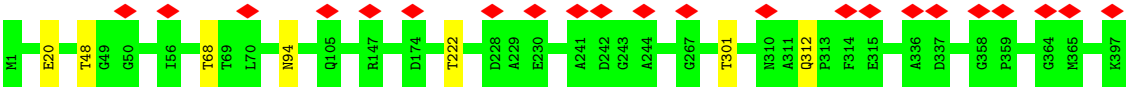
• Molecule 3: Intermediate capsid protein VP6



• Molecule 3: Intermediate capsid protein VP6

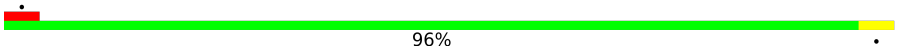


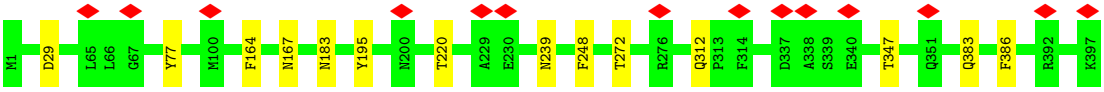
• Molecule 3: Intermediate capsid protein VP6



• Molecule 3: Intermediate capsid protein VP6

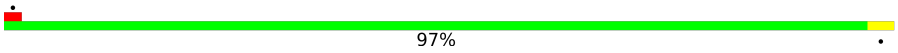
Chain l:

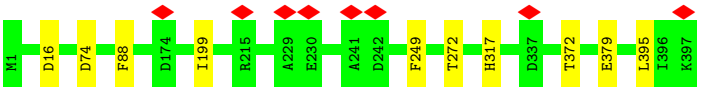




• Molecule 3: Intermediate capsid protein VP6

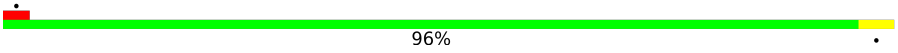
Chain m:

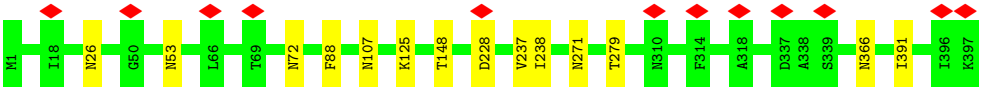




• Molecule 3: Intermediate capsid protein VP6

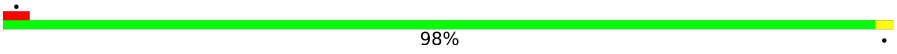
Chain n:

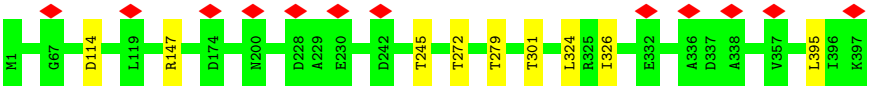




• Molecule 3: Intermediate capsid protein VP6

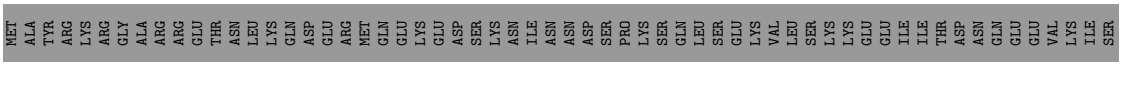
Chain o:

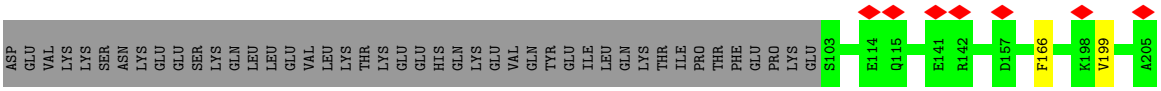


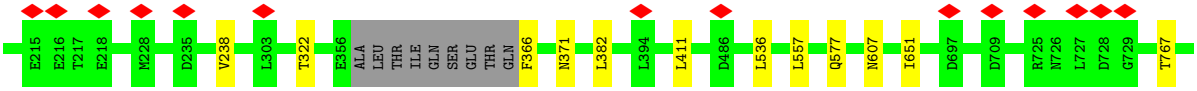


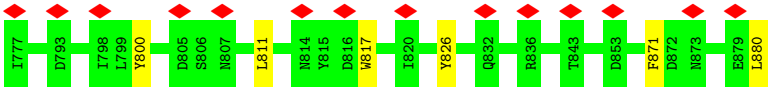
• Molecule 4: Inner capsid protein VP2

Chain q:

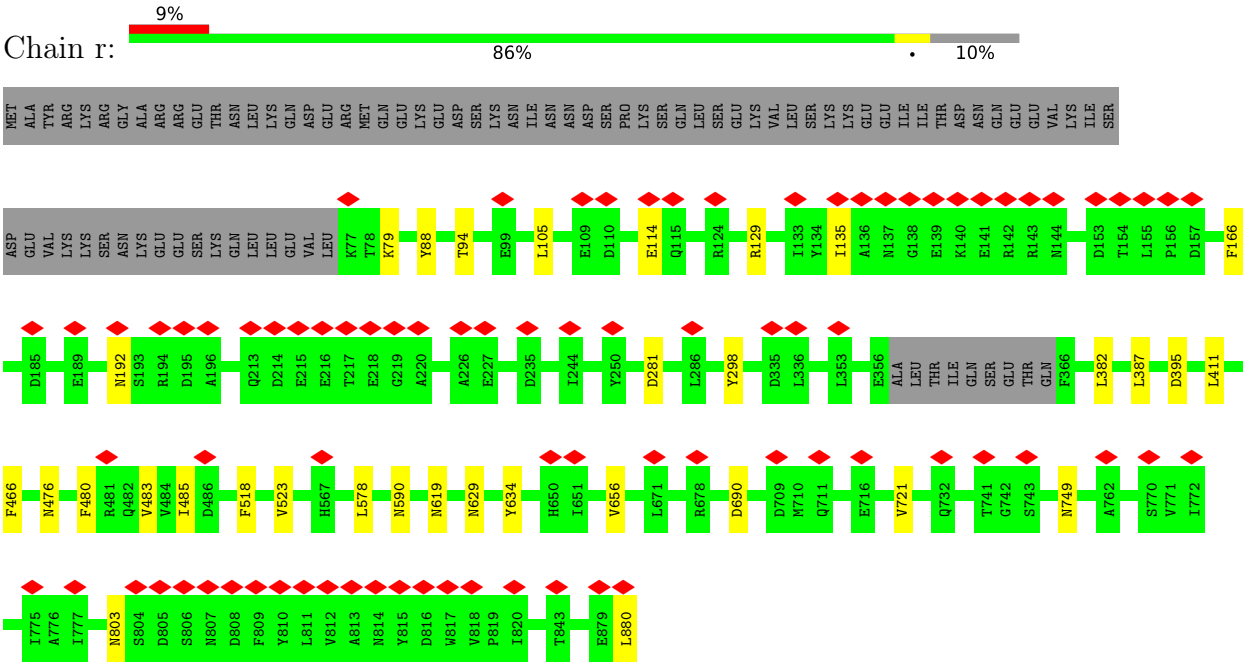








• Molecule 4: Inner capsid protein VP2



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (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	A	642/689 (93%)	617 (96%)	25 (4%)	32	57
1	B	659/689 (96%)	641 (97%)	18 (3%)	44	66
1	C	615/689 (89%)	595 (97%)	20 (3%)	38	61
2	D	235/296 (79%)	229 (97%)	6 (3%)	46	67
2	E	221/296 (75%)	214 (97%)	7 (3%)	39	62
2	F	239/296 (81%)	233 (98%)	6 (2%)	47	68
2	G	240/296 (81%)	235 (98%)	5 (2%)	53	72
2	H	219/296 (74%)	212 (97%)	7 (3%)	39	62
2	I	238/296 (80%)	231 (97%)	7 (3%)	42	64
2	J	238/296 (80%)	231 (97%)	7 (3%)	42	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	K	231/296 (78%)	228 (99%)	3 (1%)	69 82
2	L	238/296 (80%)	234 (98%)	4 (2%)	60 78
2	M	239/296 (81%)	234 (98%)	5 (2%)	53 72
2	N	237/296 (80%)	230 (97%)	7 (3%)	41 63
2	O	238/296 (80%)	228 (96%)	10 (4%)	30 55
3	d	351/351 (100%)	341 (97%)	10 (3%)	43 65
3	e	351/351 (100%)	341 (97%)	10 (3%)	43 65
3	f	351/351 (100%)	344 (98%)	7 (2%)	55 73
3	g	351/351 (100%)	345 (98%)	6 (2%)	60 78
3	h	351/351 (100%)	344 (98%)	7 (2%)	55 73
3	i	351/351 (100%)	346 (99%)	5 (1%)	67 81
3	j	351/351 (100%)	338 (96%)	13 (4%)	34 59
3	k	351/351 (100%)	344 (98%)	7 (2%)	55 73
3	l	351/351 (100%)	337 (96%)	14 (4%)	31 56
3	m	351/351 (100%)	341 (97%)	10 (3%)	43 65
3	n	351/351 (100%)	337 (96%)	14 (4%)	31 56
3	o	351/351 (100%)	342 (97%)	9 (3%)	46 67
4	q	700/809 (86%)	680 (97%)	20 (3%)	42 64
4	r	726/809 (90%)	693 (96%)	33 (4%)	27 53
All	All	10367/11449 (90%)	10065 (97%)	302 (3%)	45 64

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	n	125	LYS
4	r	480	PHE
3	n	366	ASN
4	q	607	ASN
4	r	803	ASN

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

Mol	Chain	Res	Type
3	n	381	ASN

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Mol	Chain	Res	Type
4	r	246	HIS
4	r	746	GLN
4	r	609	ASN
2	K	308	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

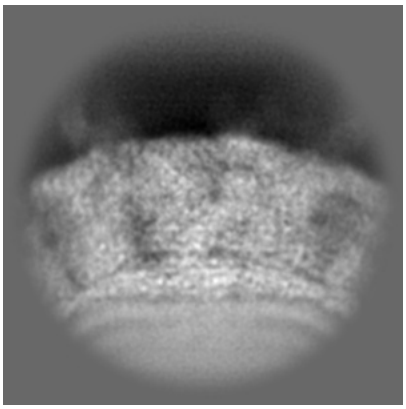
6 Map visualisation

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.

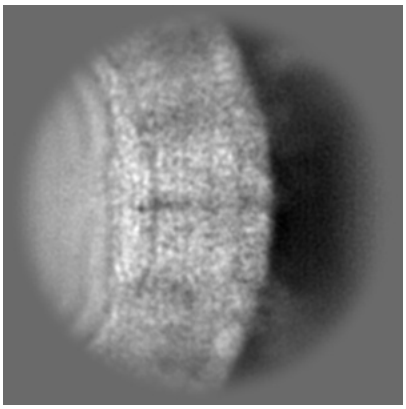
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

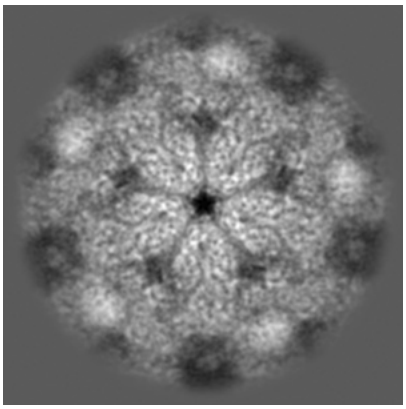
6.1.1 Primary map



X

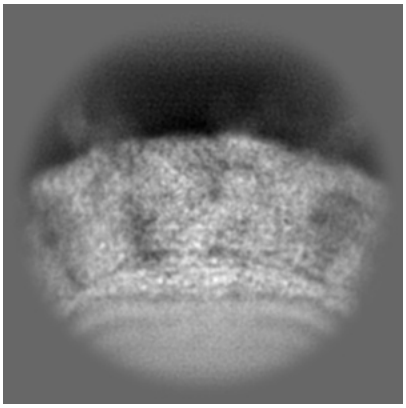


Y

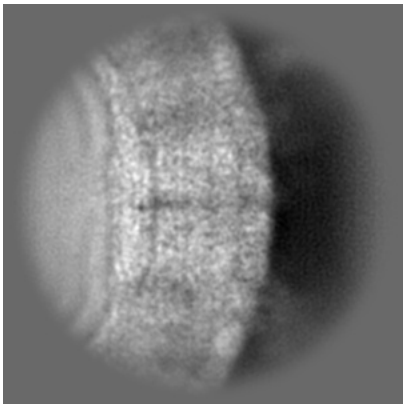


Z

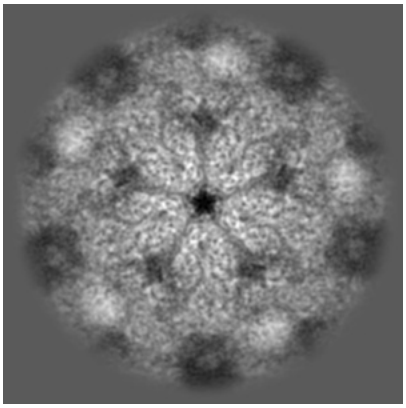
6.1.2 Raw map



X



Y

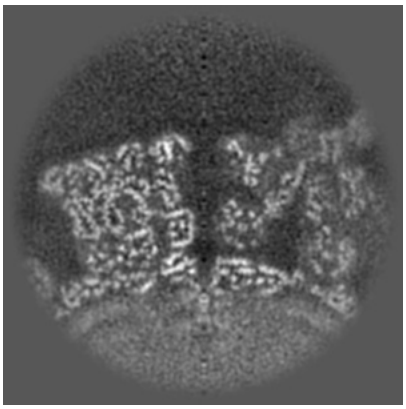


Z

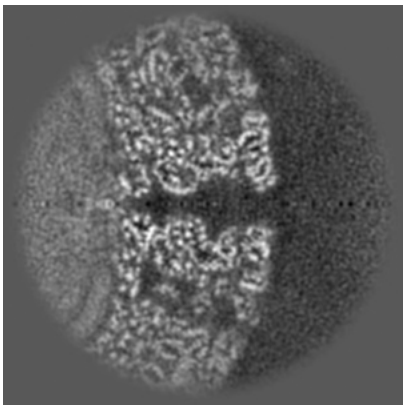
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

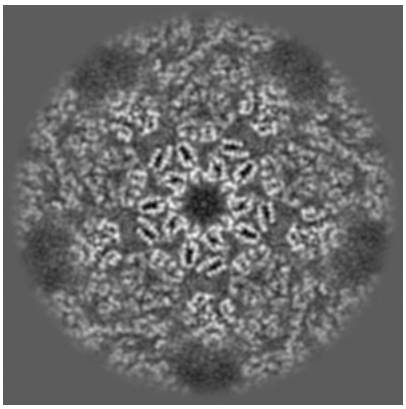
6.2.1 Primary map



X Index: 105

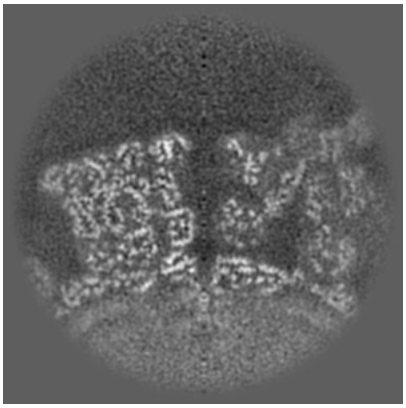


Y Index: 105

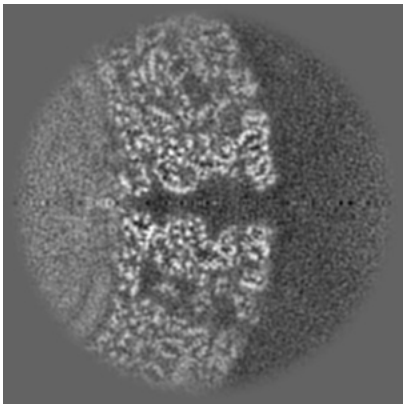


Z Index: 105

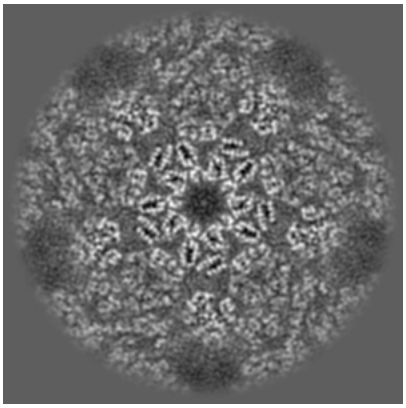
6.2.2 Raw map



X Index: 105



Y Index: 105

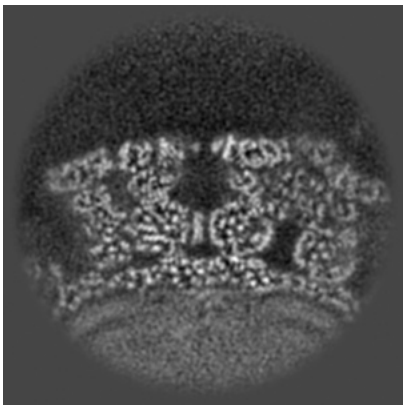


Z Index: 105

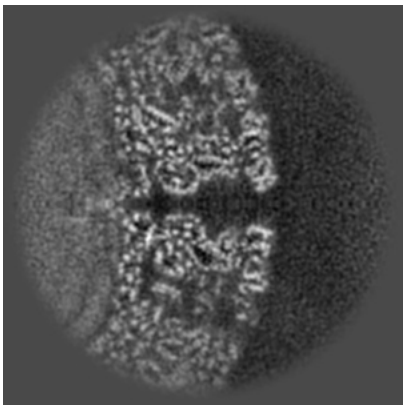
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

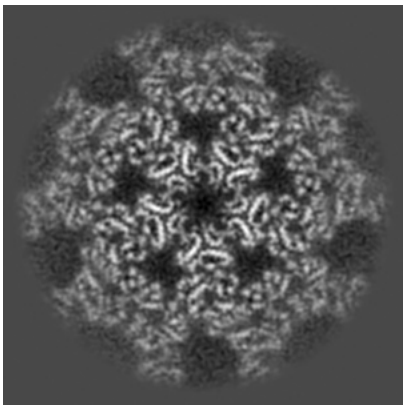
6.3.1 Primary map



X Index: 99

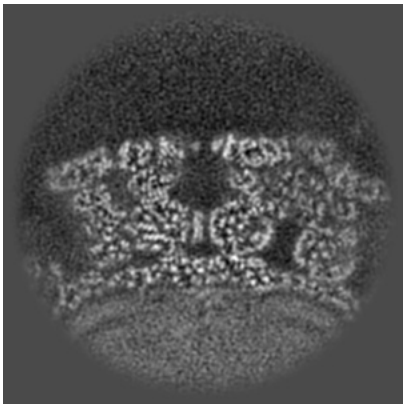


Y Index: 104

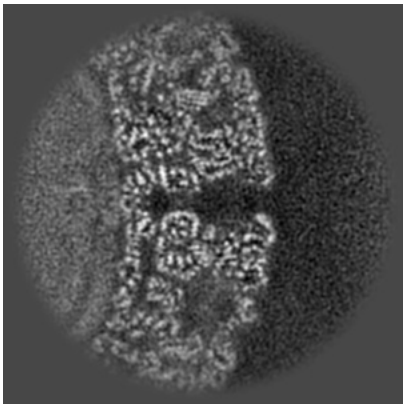


Z Index: 82

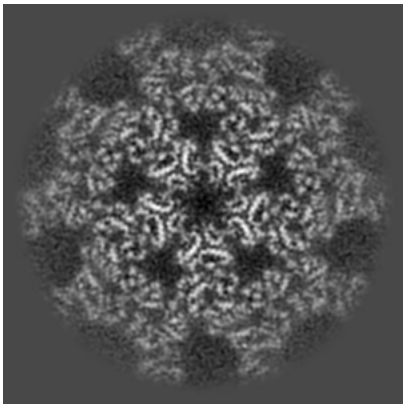
6.3.2 Raw map



X Index: 99



Y Index: 101

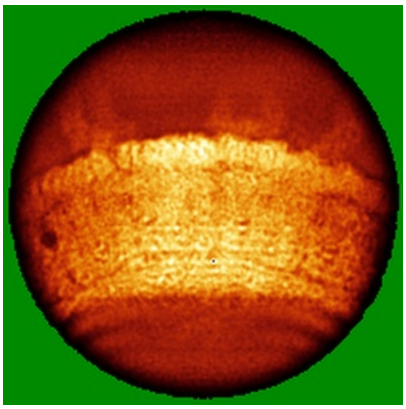


Z Index: 82

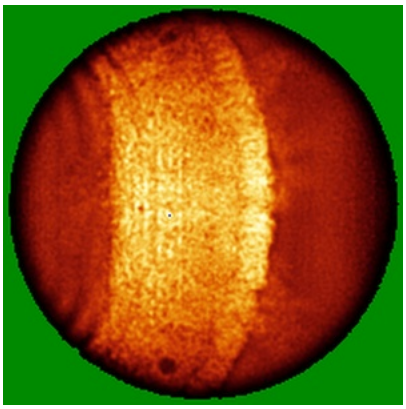
The images above show the largest variance slices of the map in three orthogonal directions.

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

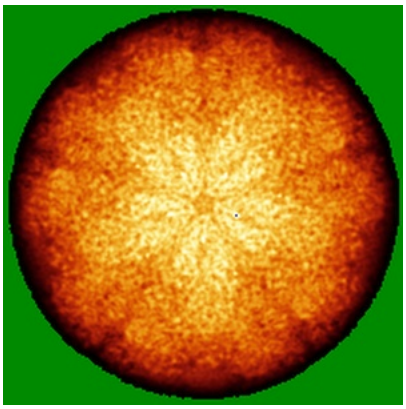
6.4.1 Primary map



X

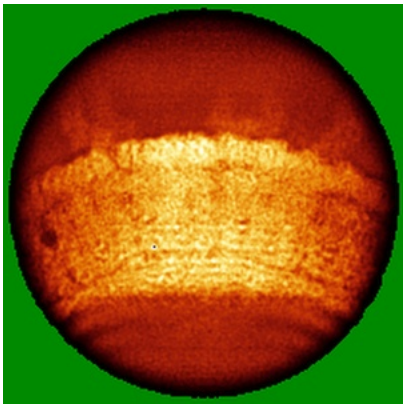


Y

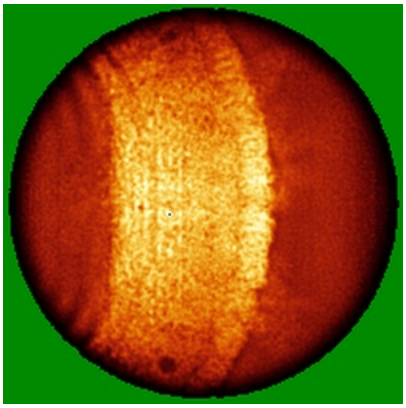


Z

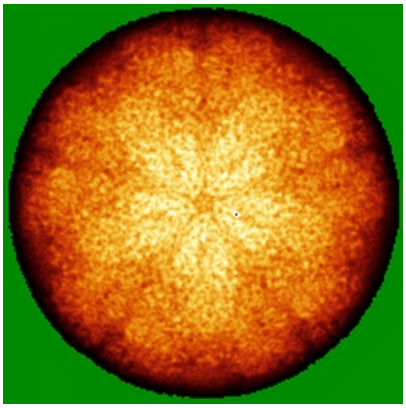
6.4.2 Raw map



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

X Y Z

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

6.5.2 Raw map

X Y Z

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

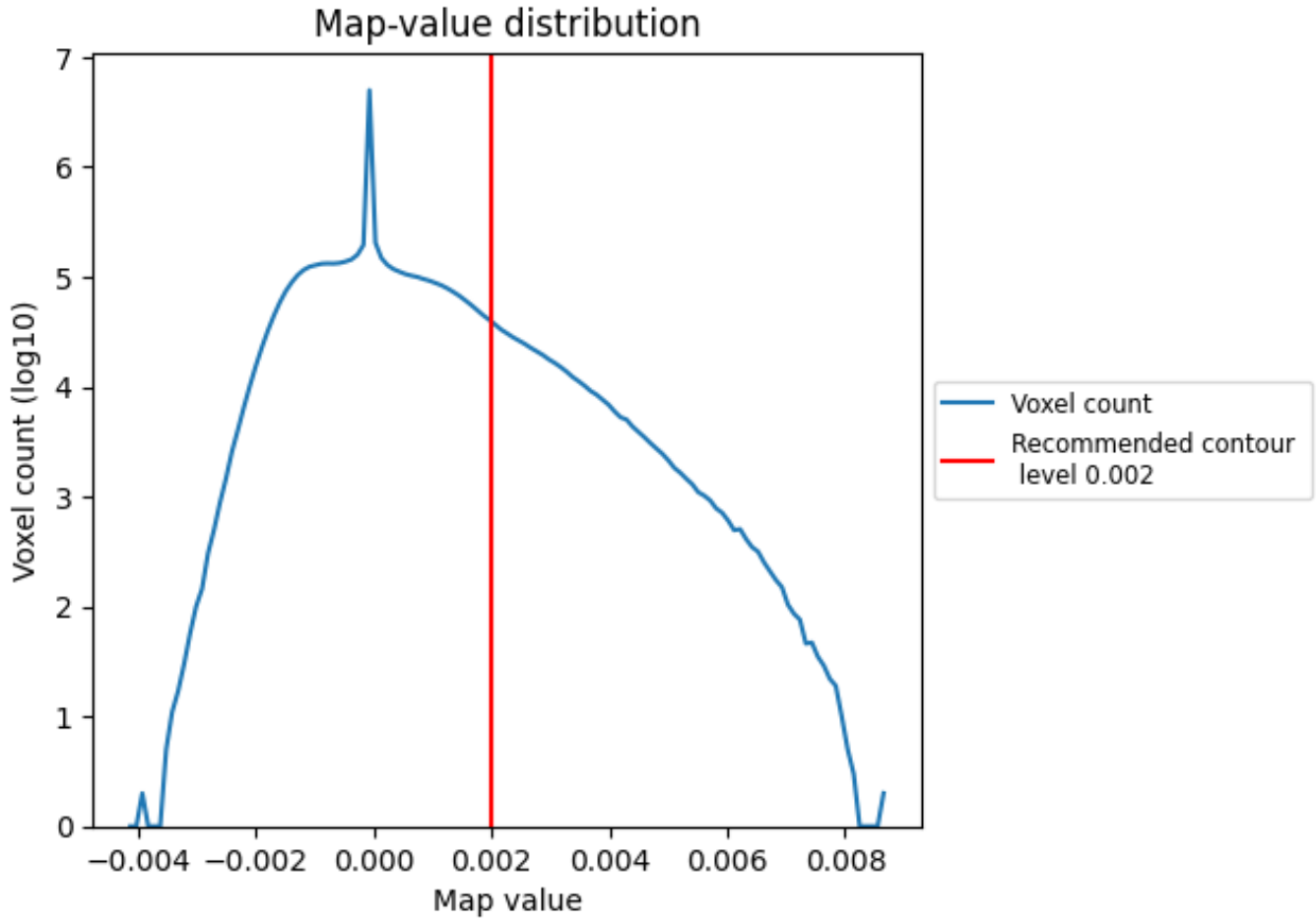
6.6 Mask visualisation (i)

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

7 Map analysis

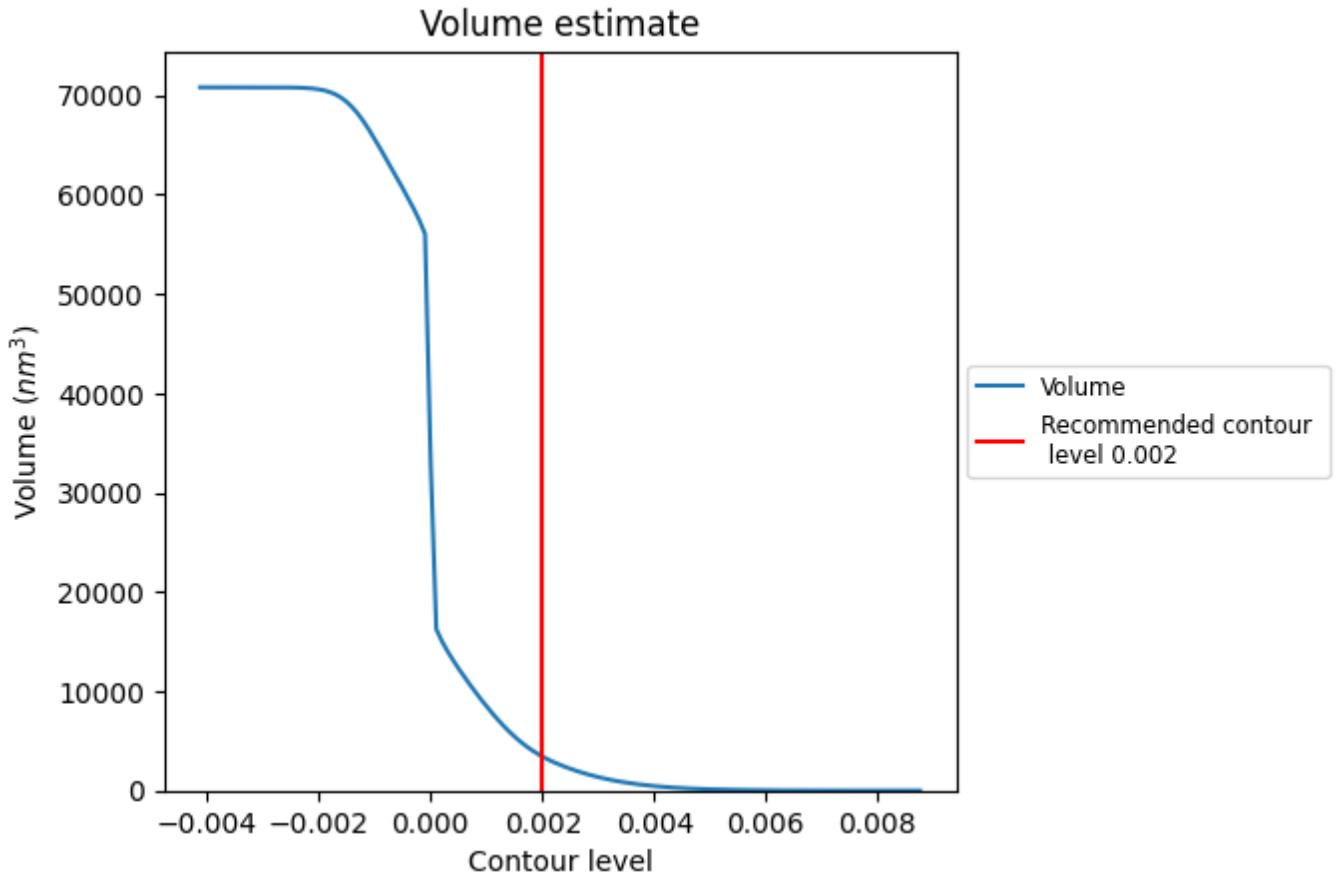
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

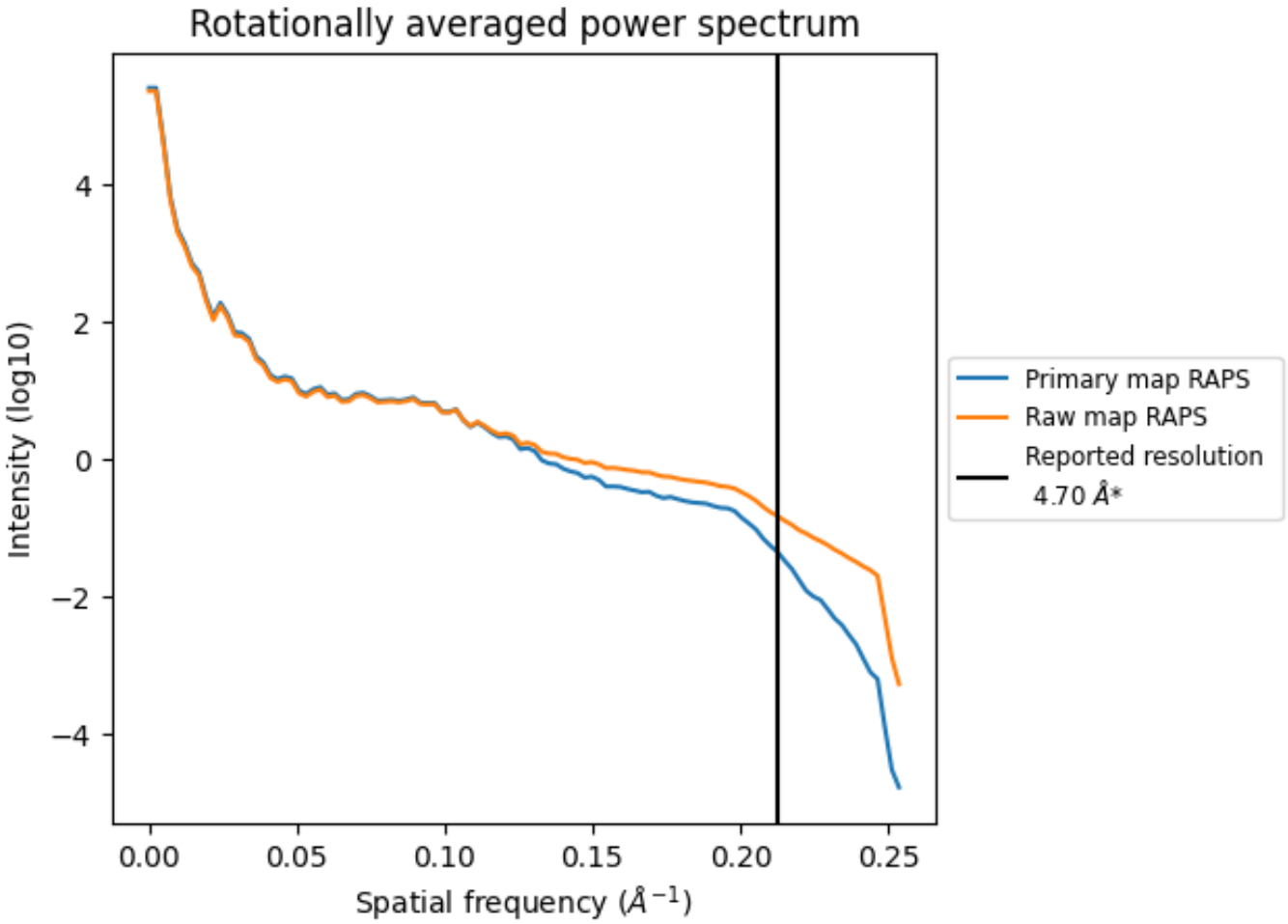
7.2 Volume estimate (i)



The volume at the recommended contour level is 3431 nm^3; 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 (i)

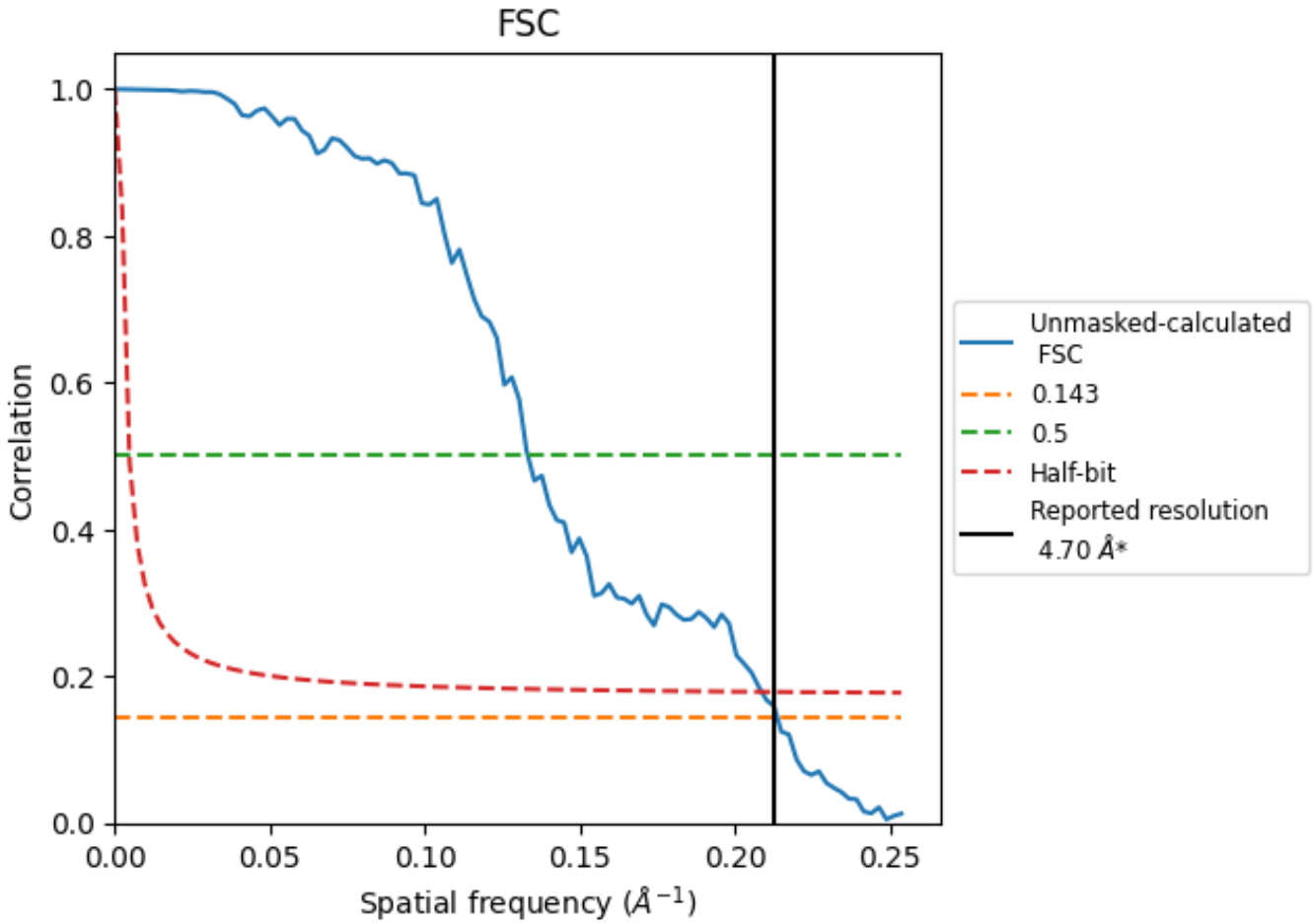


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

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 0.213 Å^{-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

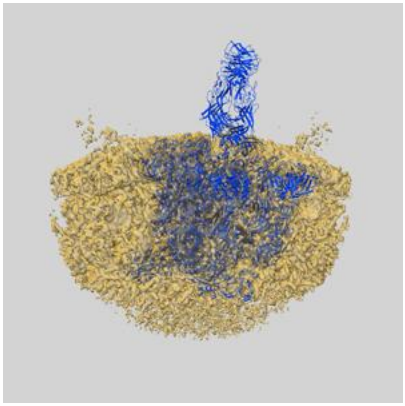
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

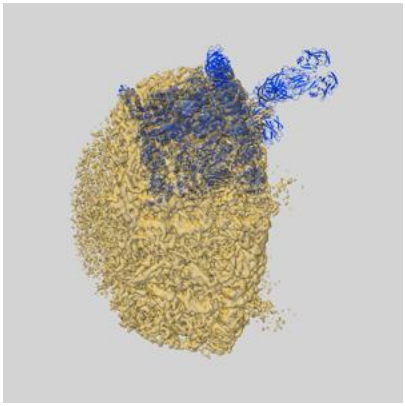
This section contains information regarding the fit between EMDB map EMD-16772 and PDB model 8CO6. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

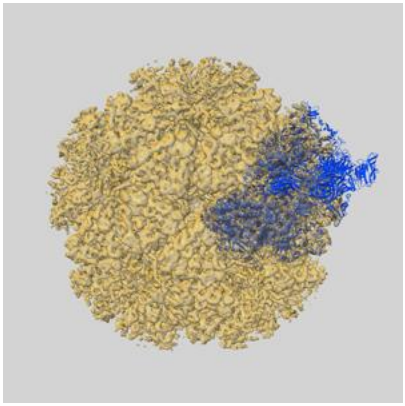
9.1.1 Map-model overlay



X

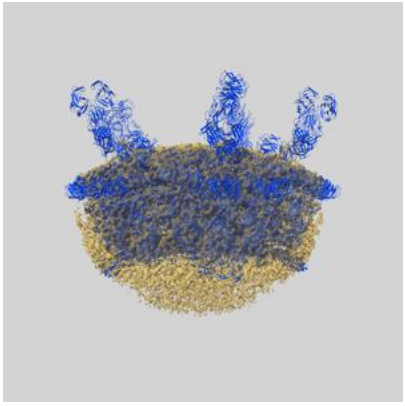


Y

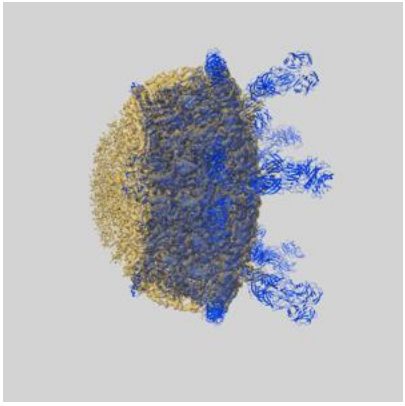


Z

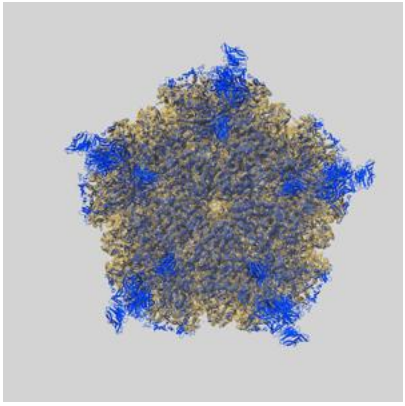
9.1.2 Map-model assembly overlay



X



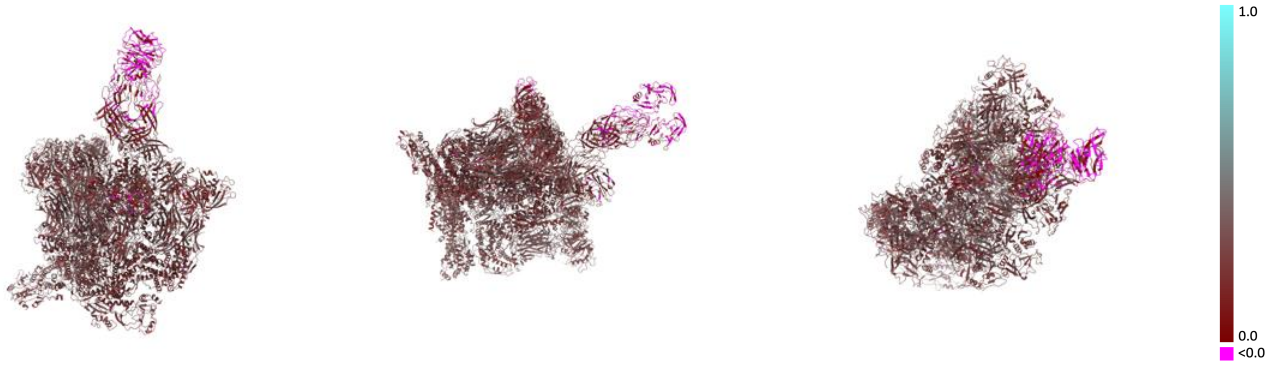
Y



Z

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

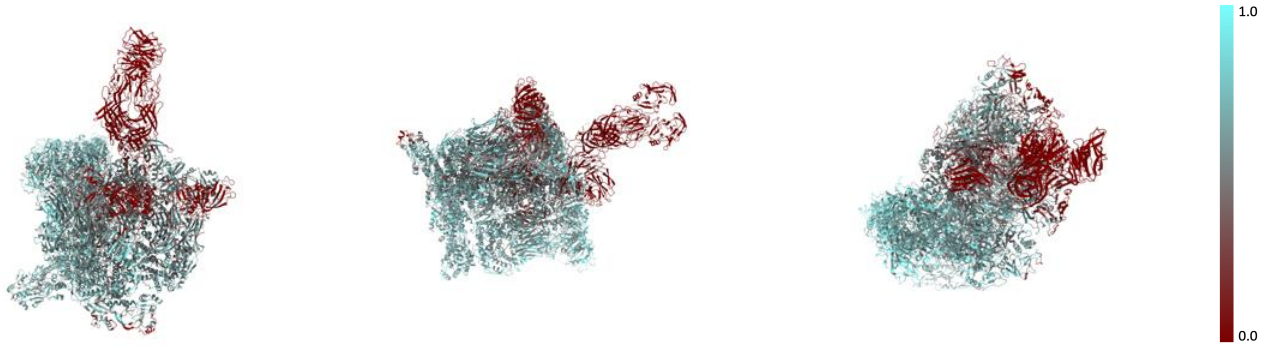
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

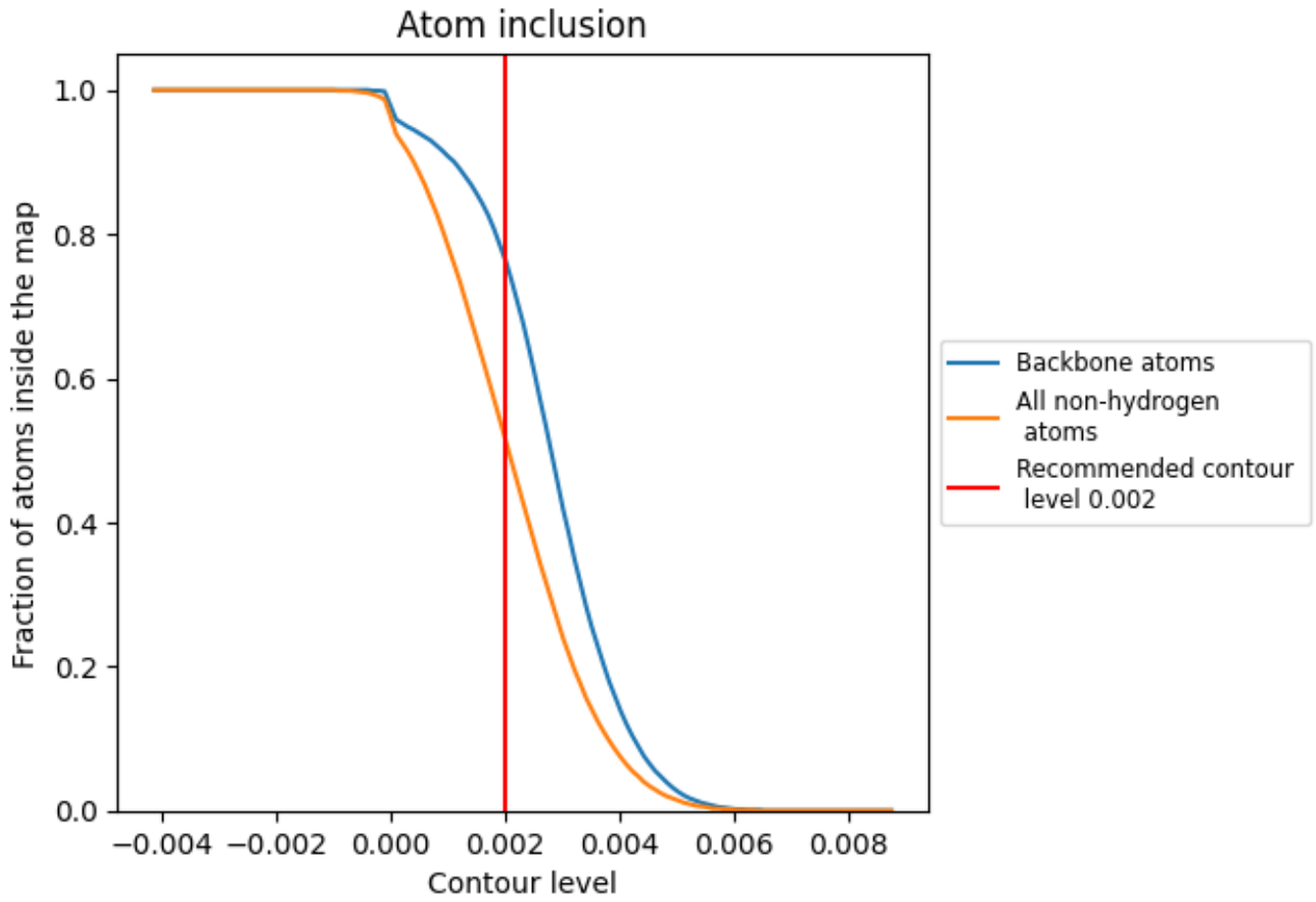
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 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