



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 11:10 PM UTC

PDB ID : 8TET / pdb_00008tet
EMDB ID : EMD-41201
Title : Human cytomegalovirus portal vertex, non-infectious enveloped particle (NIEP) configuration 1 (NC1)
Authors : Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on : 2023-07-07
Resolution : 4.26 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

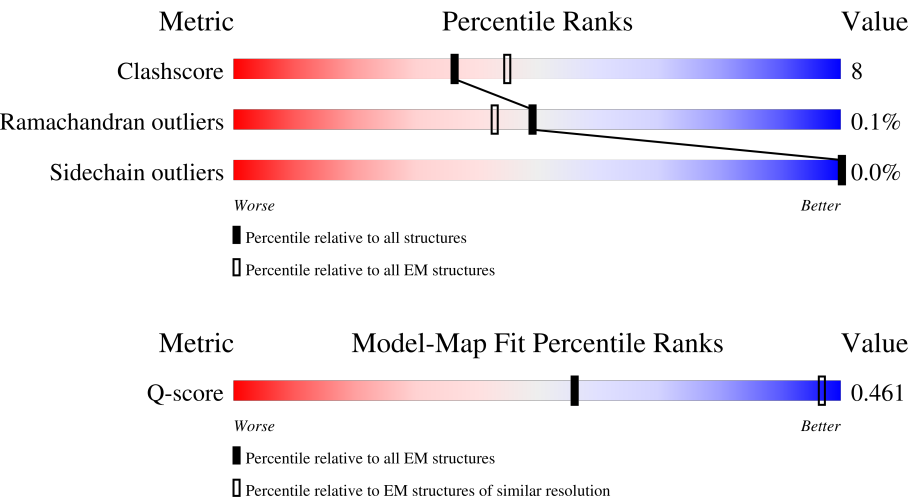
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.26 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4601 (3.76 - 4.76)

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	2241	98%
1	C	2241	98%
2	E	642	11% 10% 87%
2	F	642	12% 11% 87%

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Mol	Chain	Length	Quality of chain
3	G	594	
4	H	1370	
4	I	1370	
4	J	1370	
4	K	1370	
4	L	1370	
4	M	1370	
5	N	75	
5	O	75	
5	P	75	
5	Q	75	
5	R	75	
5	S	75	
6	T	290	
6	W	290	
7	U	306	
7	V	306	
7	X	306	
7	Y	306	
8	Z	1048	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 87998 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 Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	41	Total	C	N	O	S	0	0
			339	217	61	60	1		
1	C	40	Total	C	N	O	S	0	0
			332	213	60	58	1		

- Molecule 2 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	85	Total	C	N	O	S	0	0
			704	433	136	130	5		
2	F	86	Total	C	N	O	S	0	0
			717	445	139	129	4		

- Molecule 3 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	472	Total	C	N	O	S	0	0
			3873	2422	744	693	14		

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	1309	Total	C	N	O	S	0	0
			10391	6619	1800	1911	61		
4	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
4	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
4	K	1296	Total	C	N	O	S	0	0
			10259	6529	1787	1884	59		
4	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

- Molecule 5 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	O	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	P	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	242	Total	C	N	O	S	0	0
			1939	1248	338	342	11		
6	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	292	Total	C	N	O	S	0	0
			2317	1489	399	411	18		
7	V	288	Total	C	N	O	S	0	0
			2292	1471	397	407	17		
7	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
7	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

- Molecule 8 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		



- Molecule 1: Large tegument protein deneblyase



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



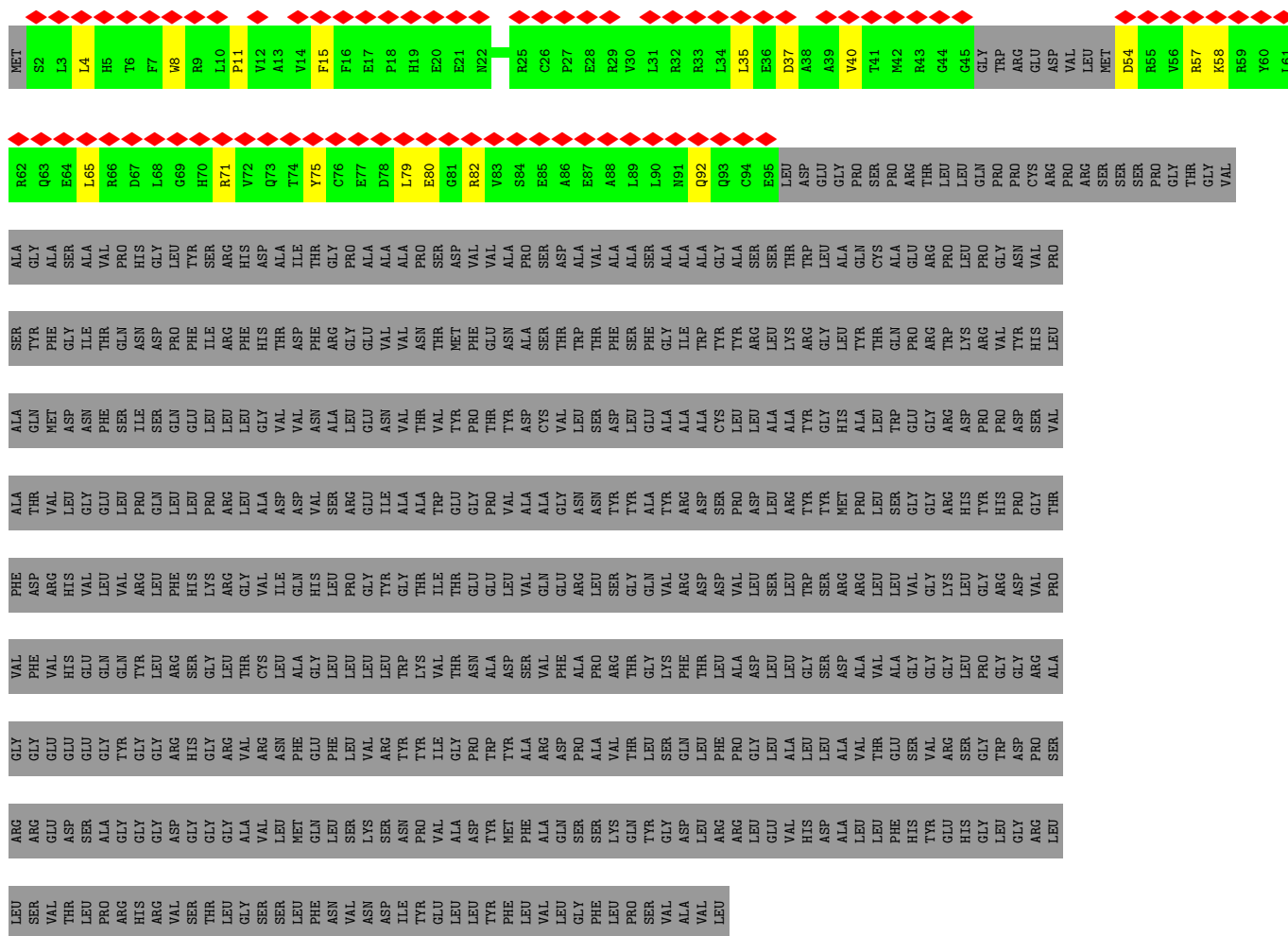
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- Molecule 2: Capsid vertex component 2

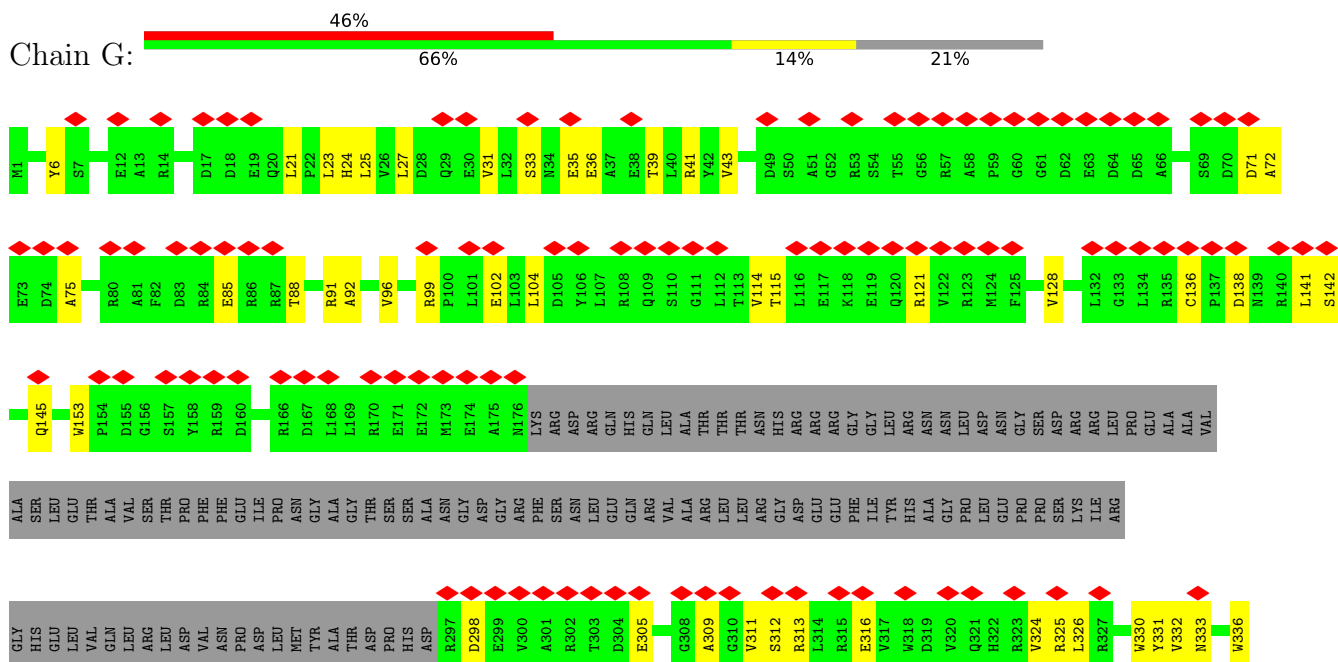
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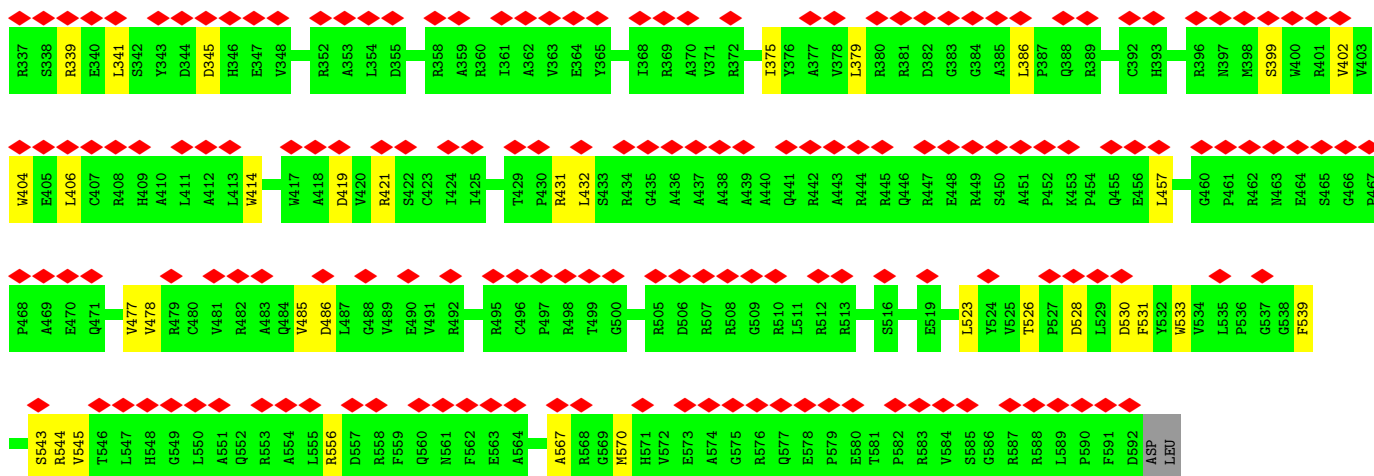
- Molecule 2: Capsid vertex component 2



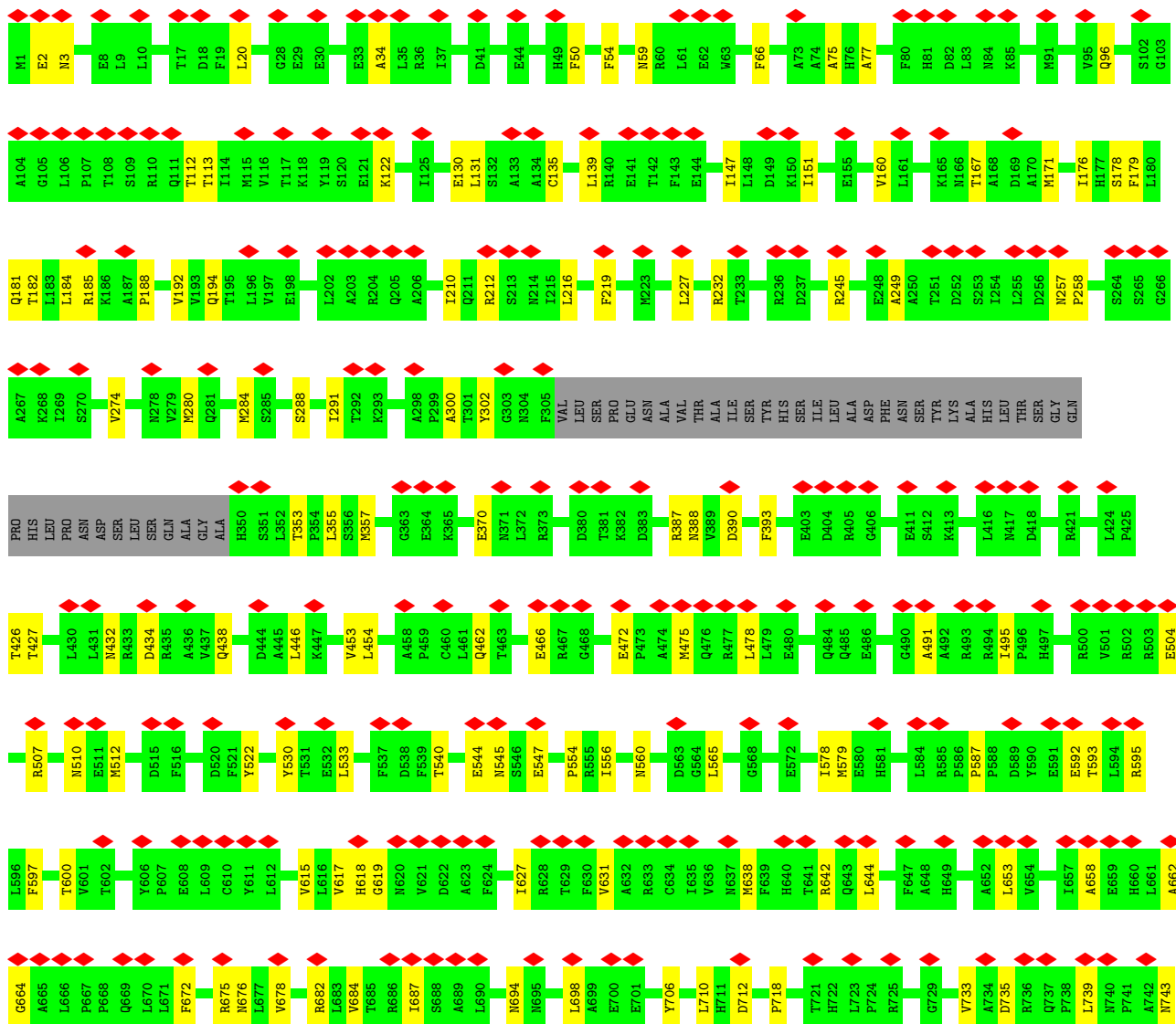
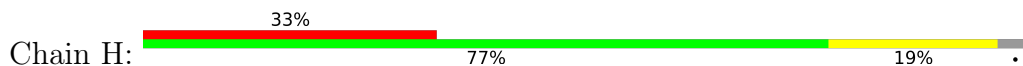


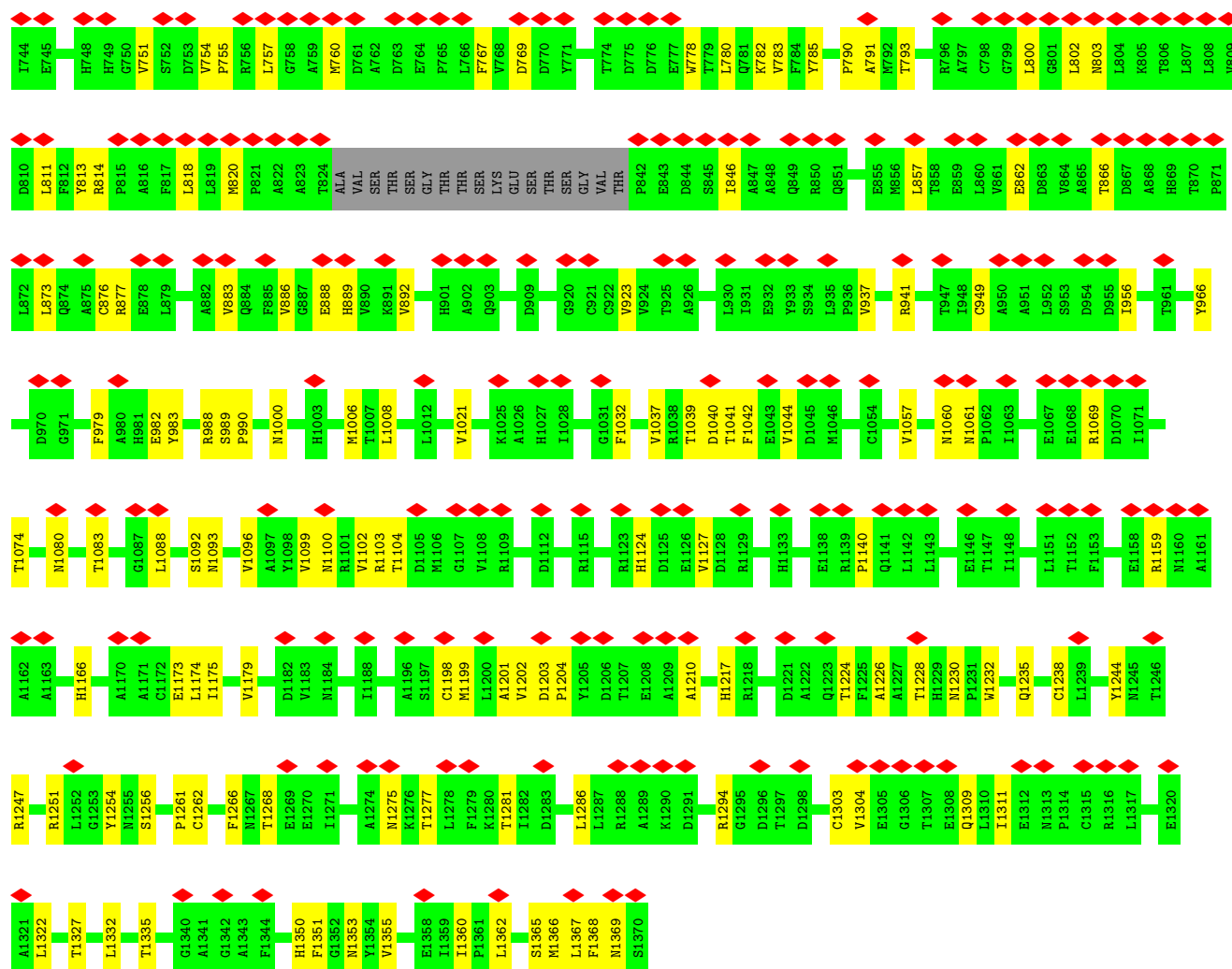
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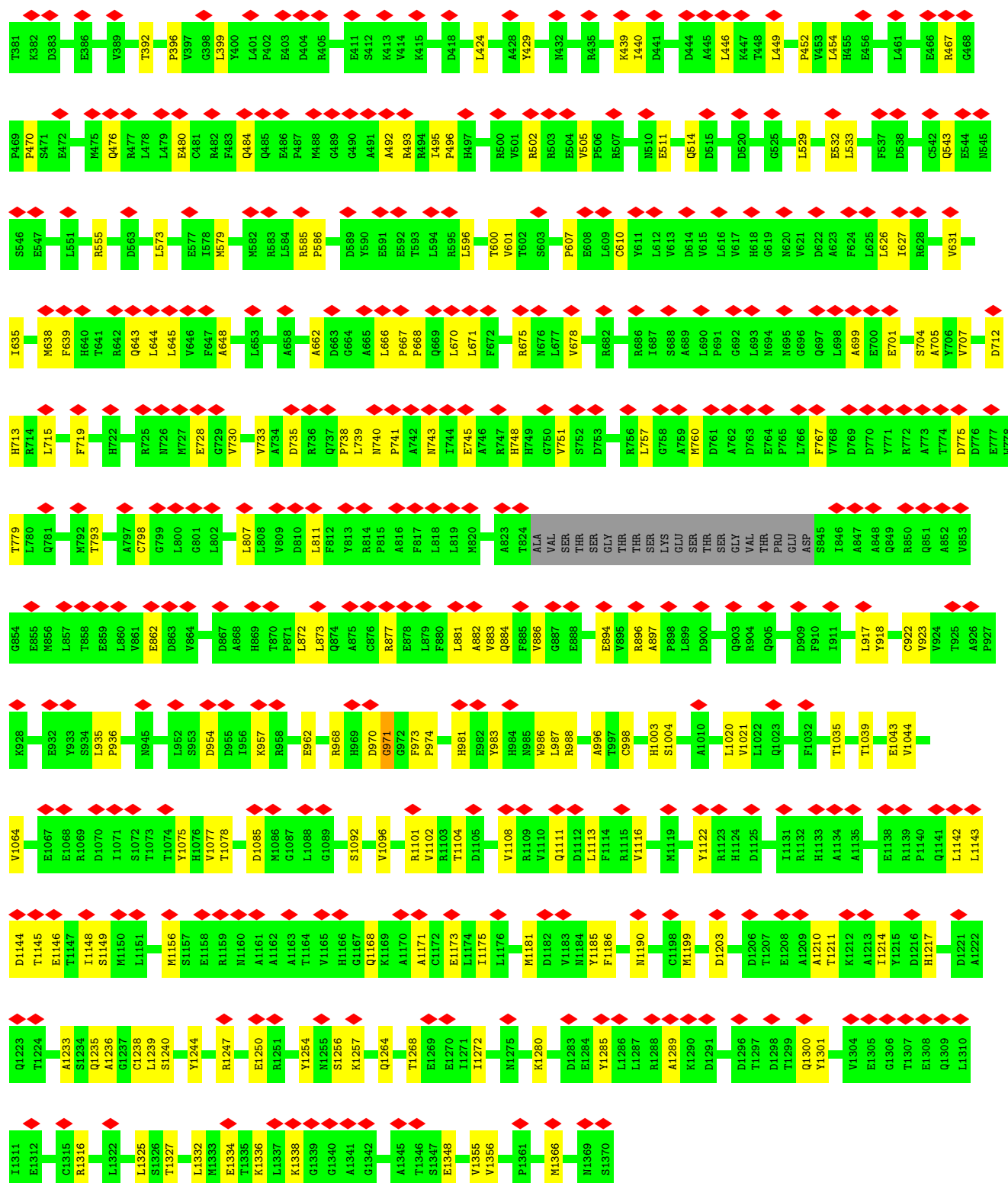




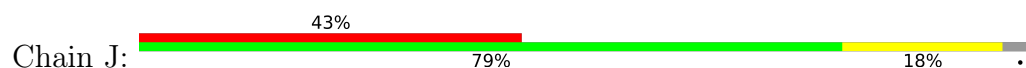
• Molecule 4: Major capsid protein



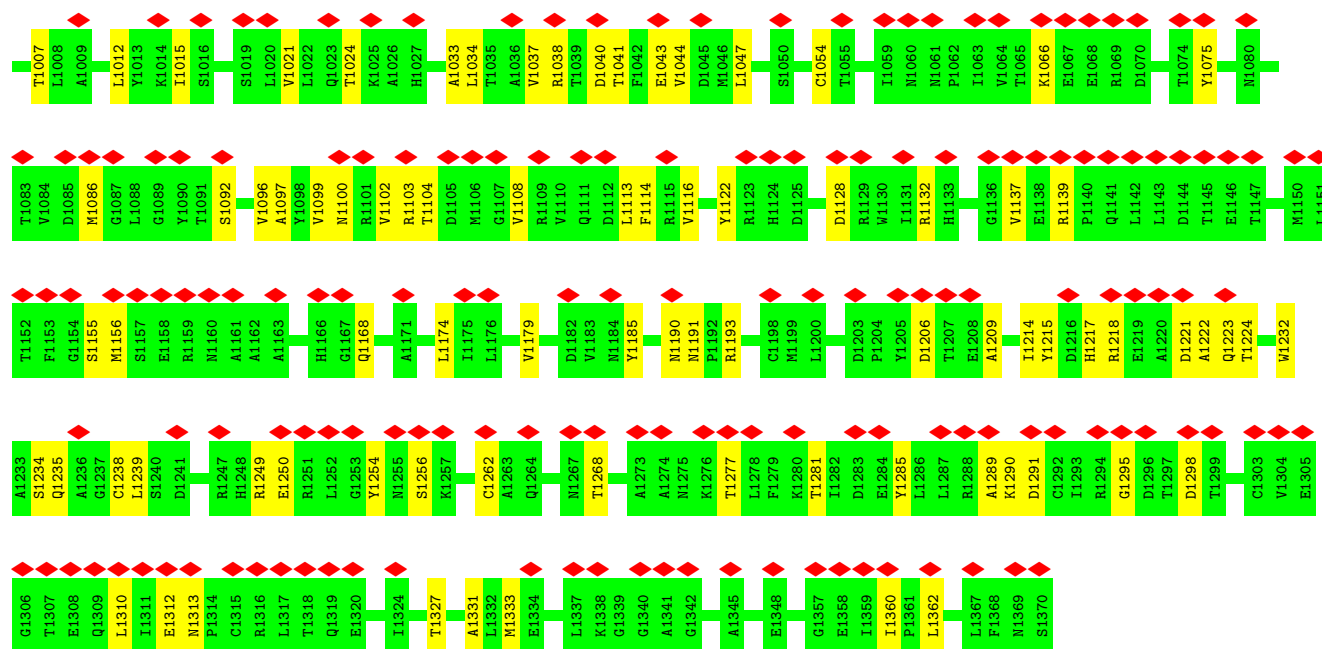




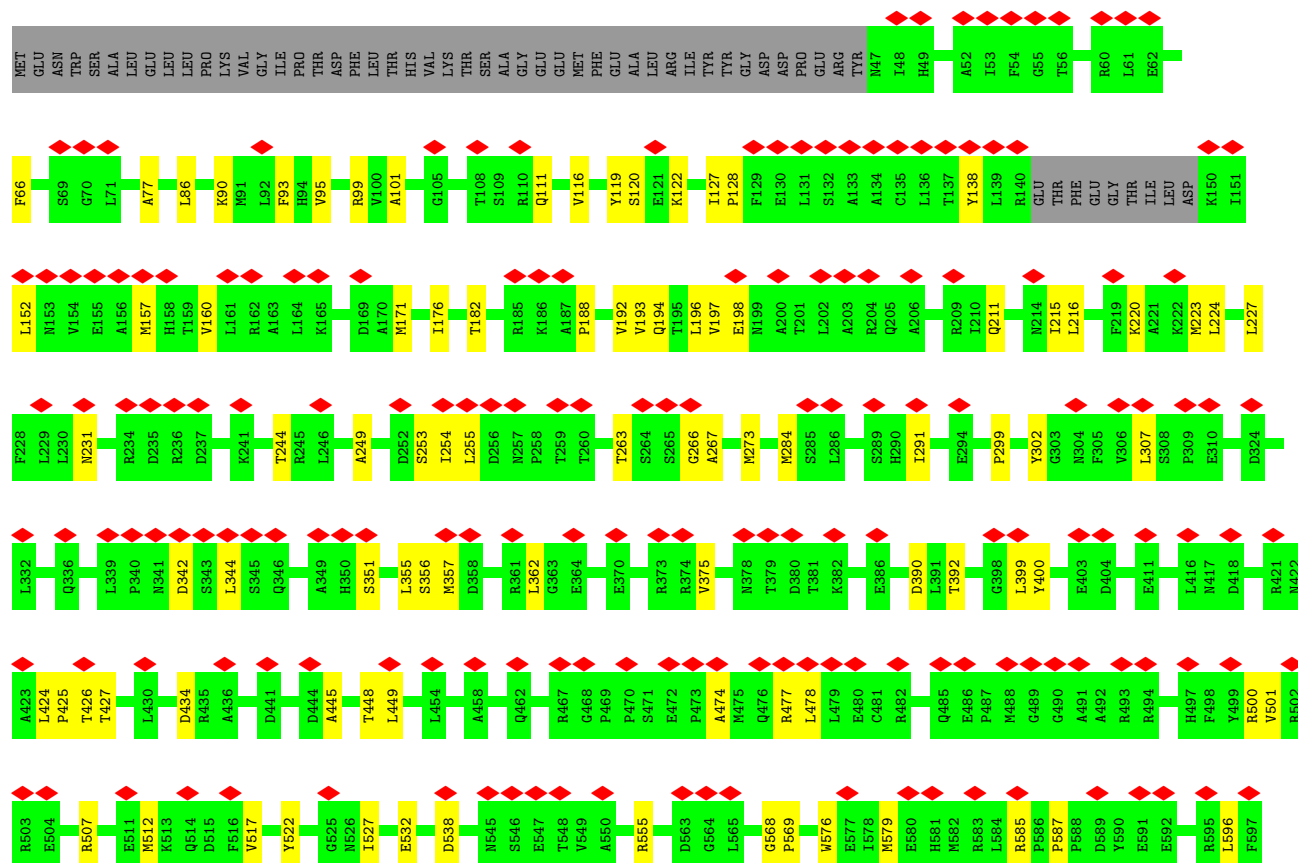
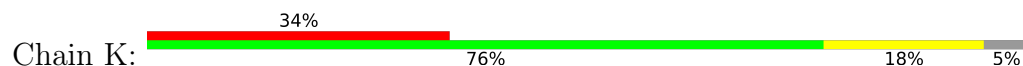
• Molecule 4: Major capsid protein

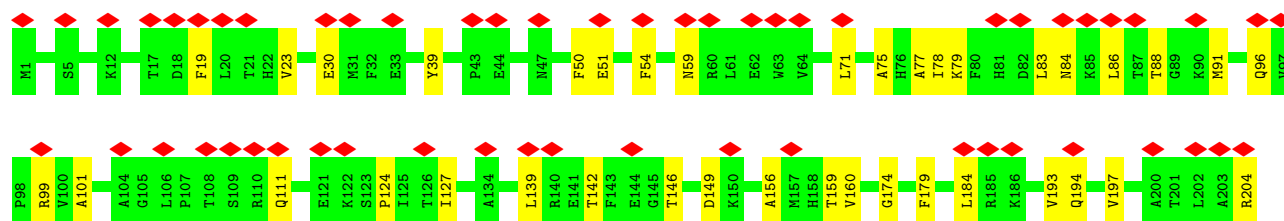




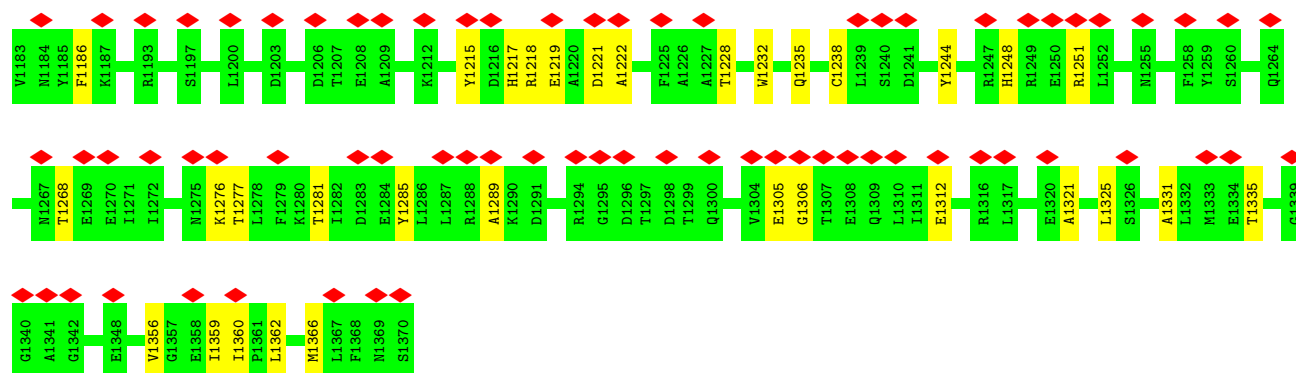


• Molecule 4: Major capsid protein

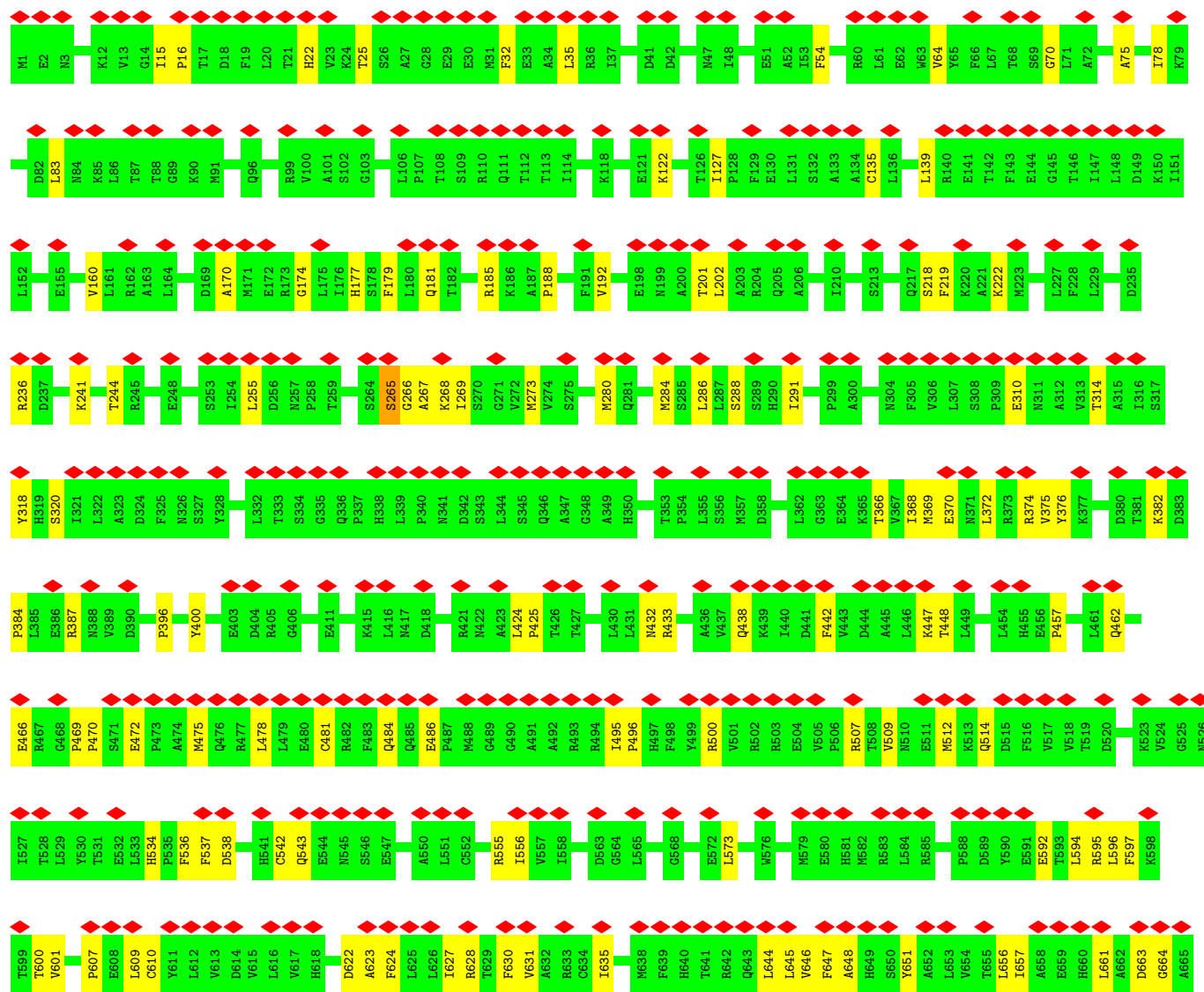
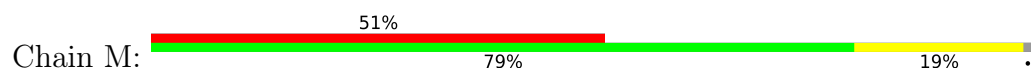


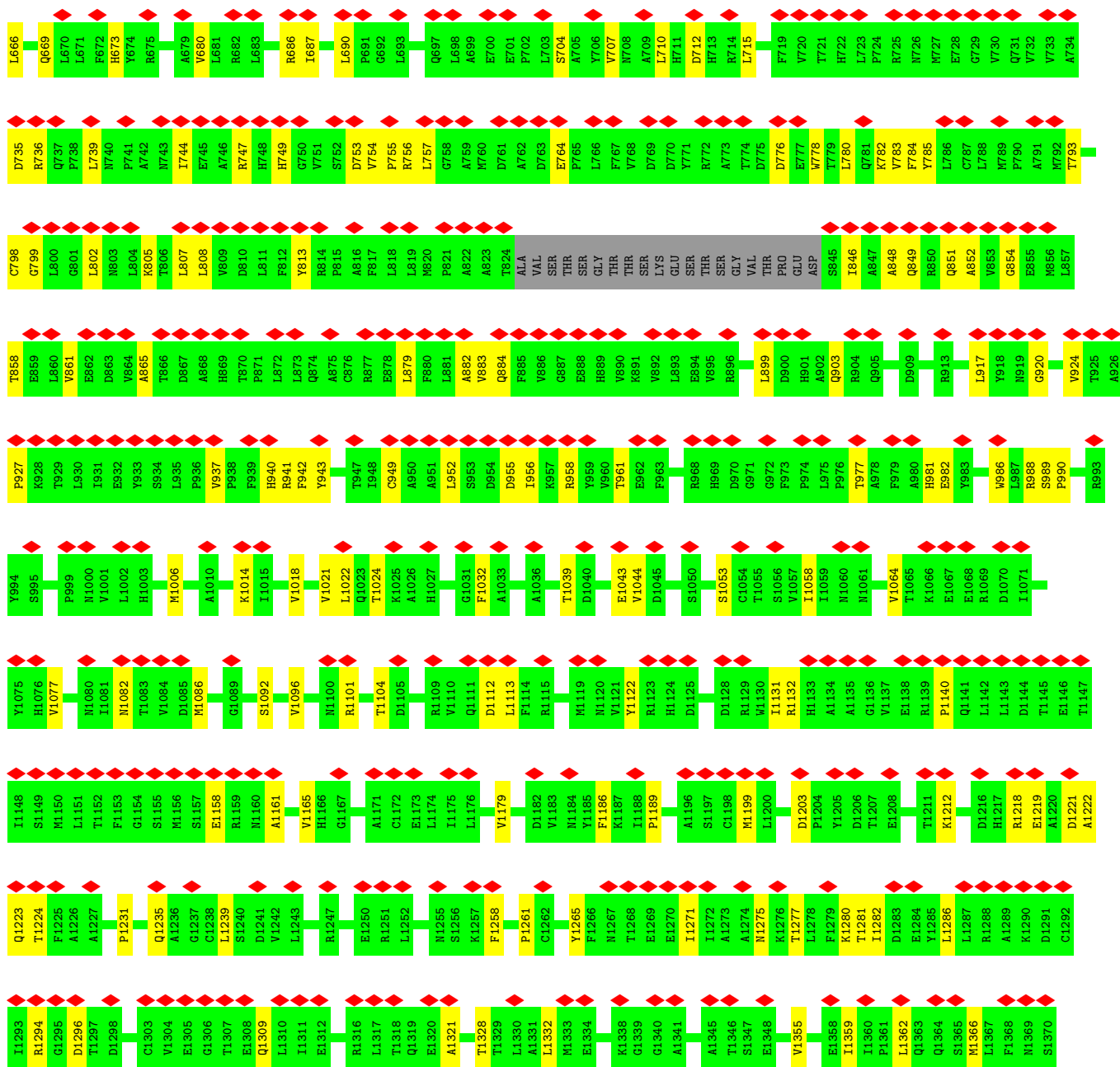




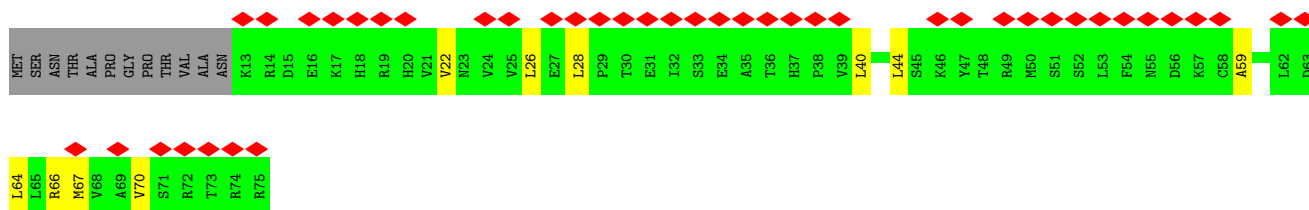


• Molecule 4: Major capsid protein

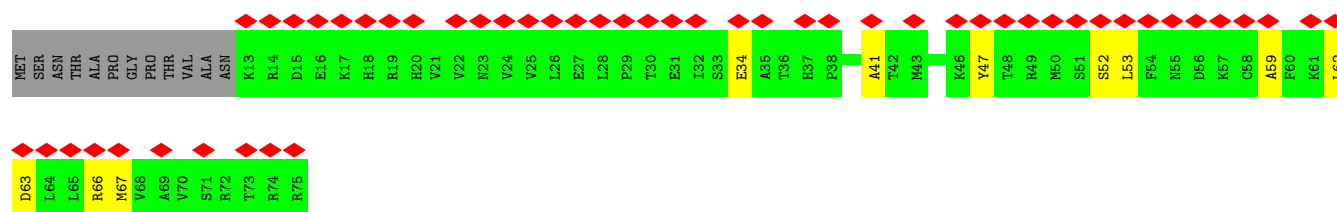
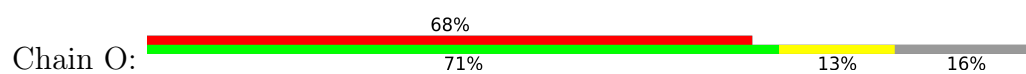




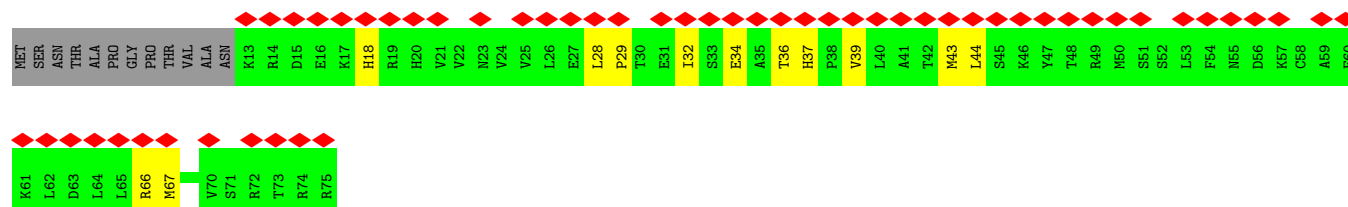
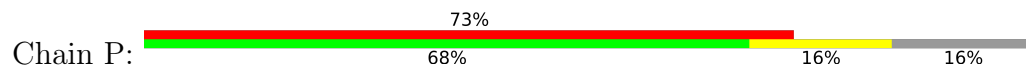
• Molecule 5: Small capsomere-interacting protein



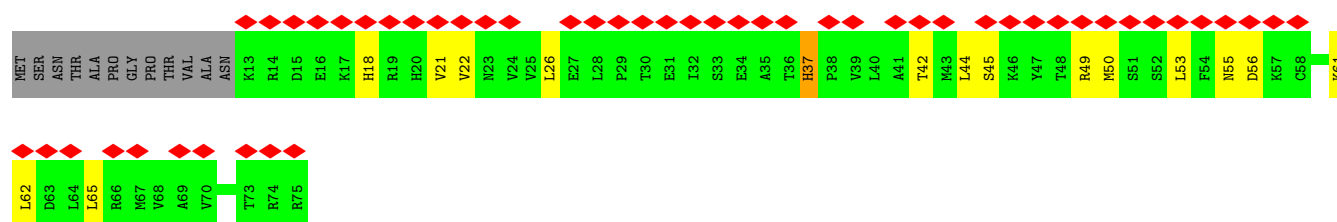
• Molecule 5: Small capsomere-interacting protein



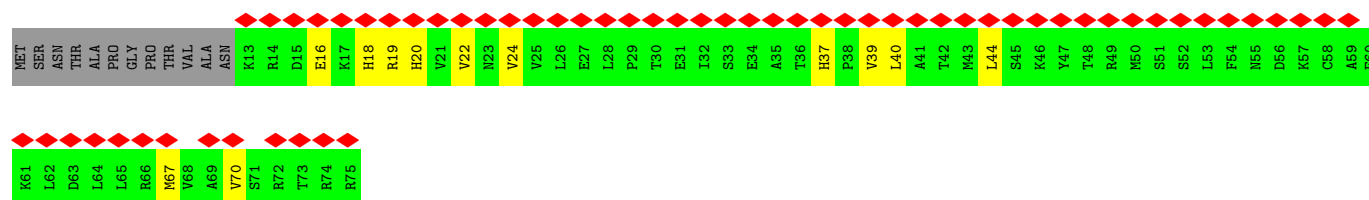
- Molecule 5: Small capsomere-interacting protein



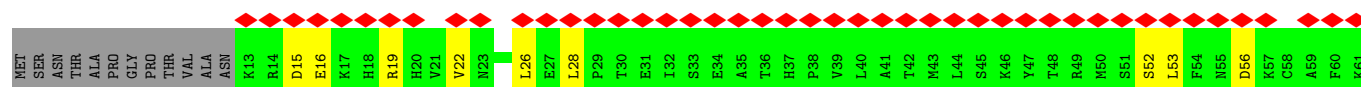
- Molecule 5: Small capsomere-interacting protein

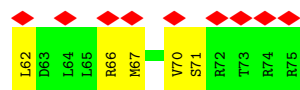


- Molecule 5: Small capsomere-interacting protein

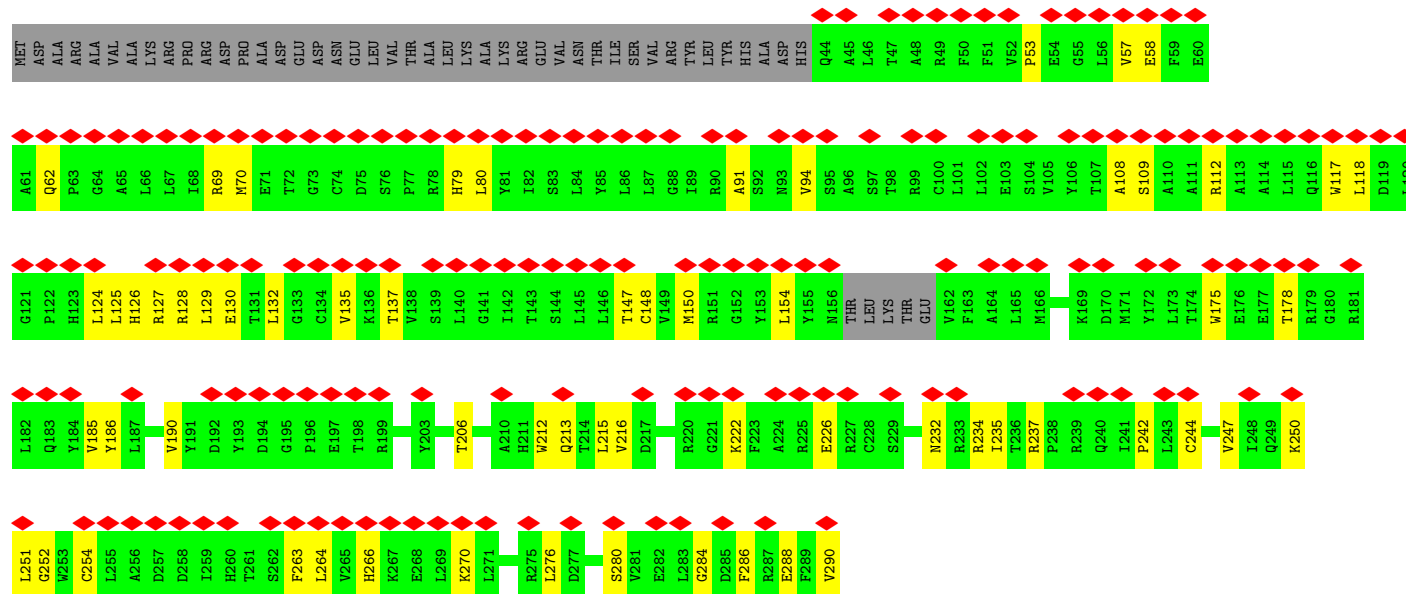


- Molecule 5: Small capsomere-interacting protein

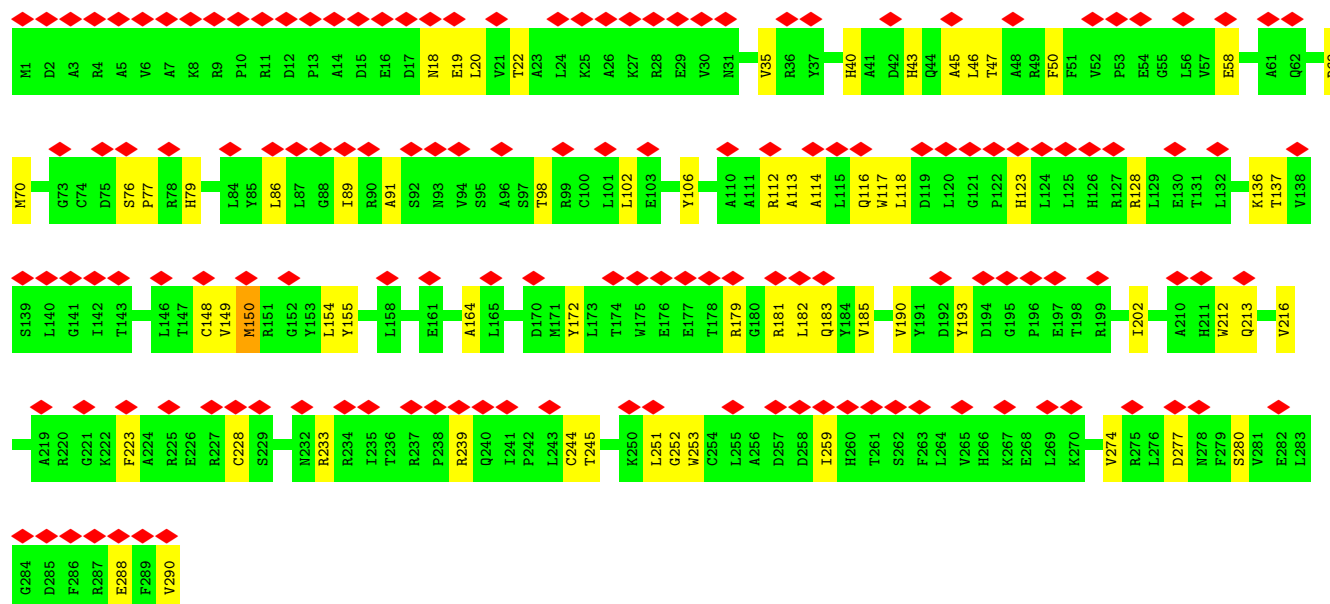
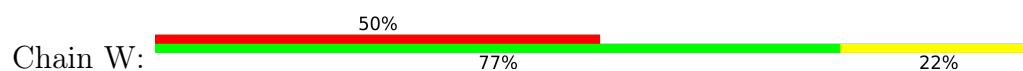




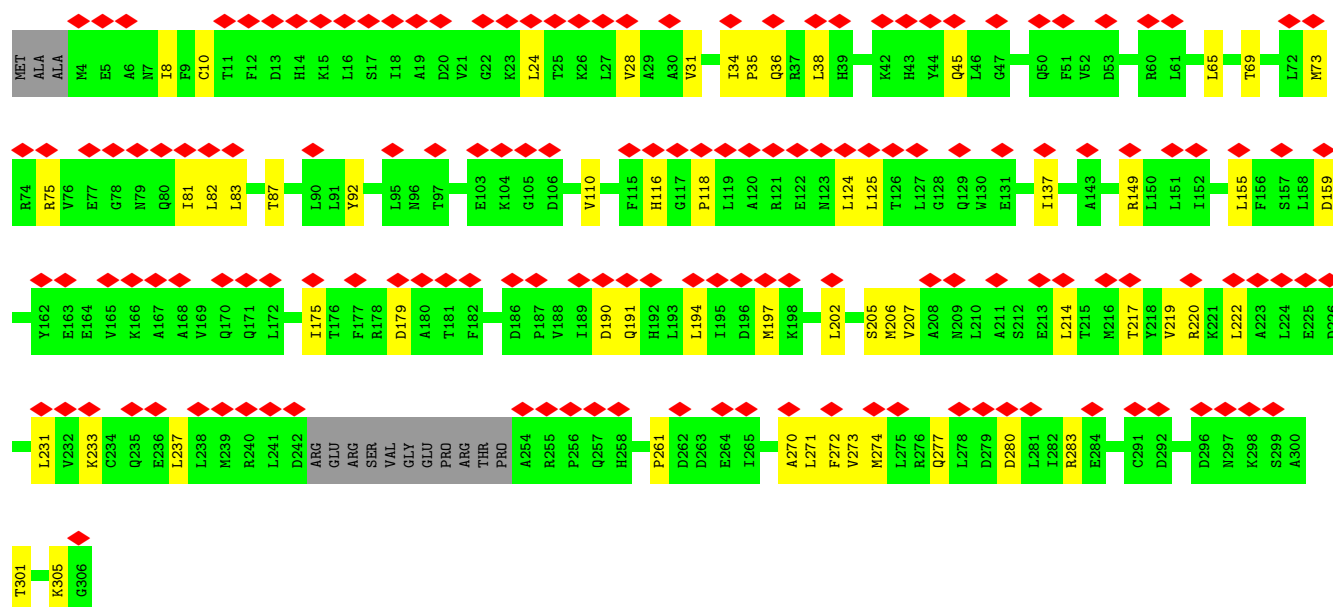
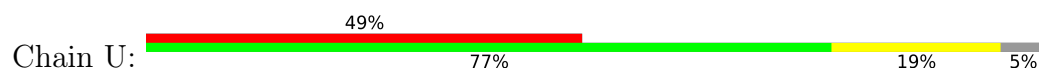
• Molecule 6: Triplex capsid protein 1



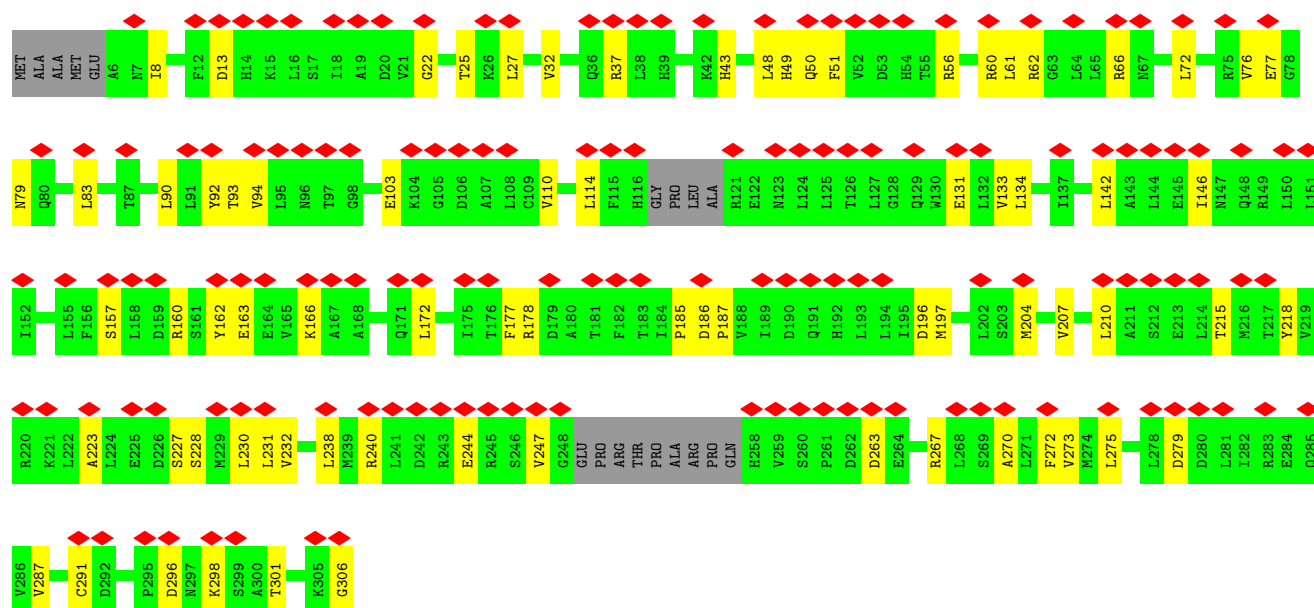
• Molecule 6: Triplex capsid protein 1



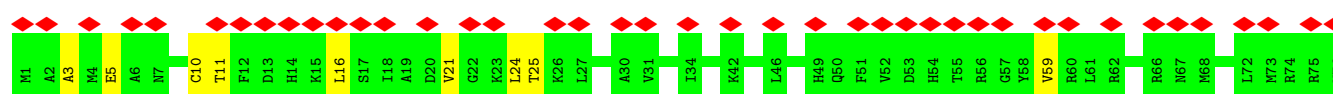
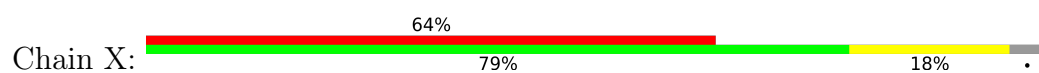
• Molecule 7: Triplex capsid protein 2

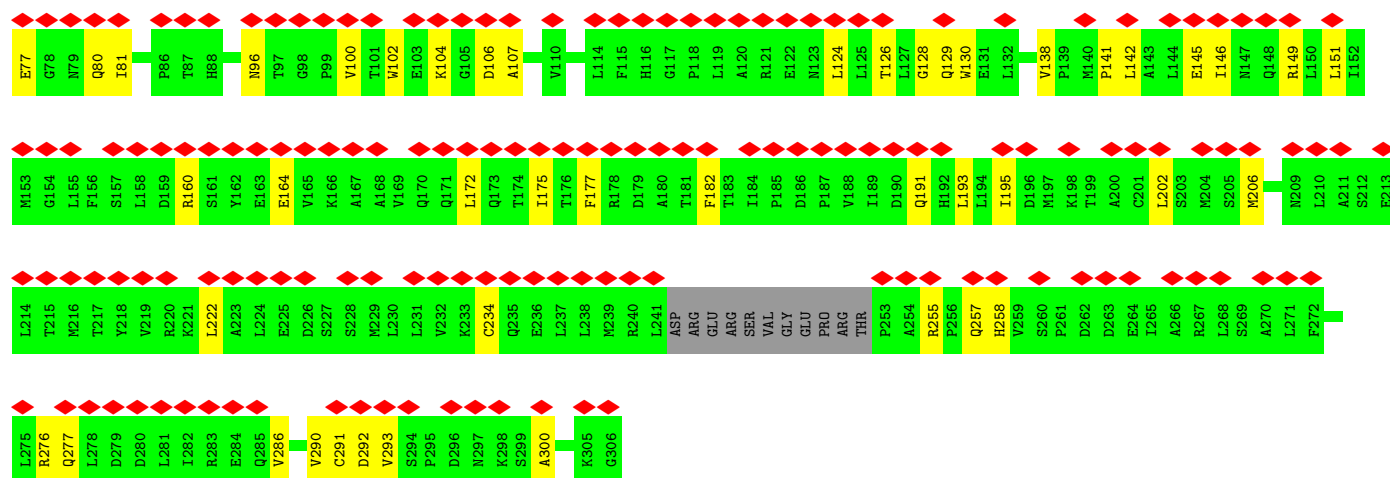


• Molecule 7: Triplex capsid protein 2

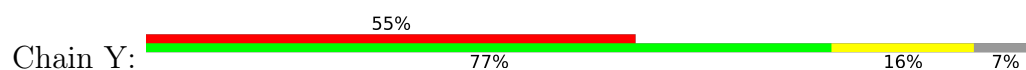


• Molecule 7: Triplex capsid protein 2





• Molecule 7: Triplex capsid protein 2



• Molecule 8: Large structural phosphoprotein



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	14020	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 ($e^-/\text{\AA}^2$)	47.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	0.15	0/341	0.36	0/460
1	C	0.15	0/334	0.41	0/450
2	E	0.15	0/713	0.34	0/958
2	F	0.14	0/728	0.33	0/979
3	G	0.17	0/3962	0.41	0/5371
4	H	0.18	0/10638	0.42	0/14487
4	I	0.17	0/10949	0.42	1/14916 (0.0%)
4	J	0.17	0/10682	0.41	0/14553
4	K	0.18	0/10503	0.42	0/14307
4	L	0.17	0/10949	0.41	2/14916 (0.0%)
4	M	0.16	0/10949	0.42	0/14916
5	N	0.13	0/520	0.36	0/697
5	O	0.13	0/520	0.35	0/697
5	P	0.13	0/520	0.35	0/697
5	Q	0.16	0/520	0.44	0/697
5	R	0.11	0/520	0.33	0/697
5	S	0.13	0/520	0.35	0/697
6	T	0.18	0/1981	0.48	0/2687
6	W	0.19	0/2374	0.50	0/3221
7	U	0.18	0/2361	0.45	0/3206
7	V	0.18	0/2333	0.45	0/3164
7	X	0.16	0/2379	0.42	0/3230
7	Y	0.17	0/2305	0.43	0/3126
8	Z	0.17	0/2358	0.42	0/3182
All	All	0.17	0/89959	0.42	3/122311 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	I	0	2
4	K	0	1
4	L	0	1
4	M	0	1
6	W	0	2
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	971	GLY	N-CA-C	-6.78	105.44	111.67
4	L	988	ARG	CA-C-N	5.38	127.68	120.58
4	L	988	ARG	C-N-CA	5.38	127.68	120.58

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	1100	ASN	Peptide
4	I	1143	LEU	Peptide
4	I	265	SER	Peptide
4	K	1100	ASN	Peptide
4	L	265	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	339	0	365	10	0
1	C	332	0	358	16	0
2	E	704	0	696	19	0
2	F	717	0	710	17	0
3	G	3873	0	3792	60	0
4	H	10391	0	10342	167	0
4	I	10693	0	10635	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	10433	0	10379	155	0
4	K	10259	0	10216	170	0
4	L	10693	0	10635	187	0
4	M	10693	0	10635	168	0
5	N	513	0	539	7	0
5	O	513	0	539	8	0
5	P	513	0	539	10	0
5	Q	513	0	539	14	0
5	R	513	0	539	7	0
5	S	513	0	539	11	0
6	T	1939	0	1972	46	0
6	W	2325	0	2363	49	0
7	U	2317	0	2405	42	0
7	V	2292	0	2379	56	0
7	X	2334	0	2431	39	0
7	Y	2266	0	2355	34	0
8	Z	2320	0	2351	31	0
All	All	87998	0	88253	1351	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1351 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:819:LEU:HD23	5:Q:37:HIS:HE1	1.33	0.93
7:Y:56:ARG:HH11	7:Y:60:ARG:HG2	1.35	0.92
4:J:1103:ARG:HH22	4:J:1295:GLY:HA2	1.35	0.91
4:J:985:ASN:O	4:J:988:ARG:NH1	2.03	0.91
3:G:457:LEU:HG	6:W:116:GLN:HE21	1.41	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	39/2241 (2%)	39 (100%)	0	0	100	100
1	C	38/2241 (2%)	37 (97%)	1 (3%)	0	100	100
2	E	83/642 (13%)	82 (99%)	1 (1%)	0	100	100
2	F	82/642 (13%)	80 (98%)	2 (2%)	0	100	100
3	G	468/594 (79%)	443 (95%)	25 (5%)	0	100	100
4	H	1303/1370 (95%)	1231 (94%)	71 (5%)	1 (0%)	48	83
4	I	1346/1370 (98%)	1272 (94%)	72 (5%)	2 (0%)	48	83
4	J	1313/1370 (96%)	1241 (94%)	71 (5%)	1 (0%)	48	83
4	K	1290/1370 (94%)	1225 (95%)	64 (5%)	1 (0%)	48	83
4	L	1346/1370 (98%)	1281 (95%)	64 (5%)	1 (0%)	48	83
4	M	1346/1370 (98%)	1273 (95%)	71 (5%)	2 (0%)	48	83
5	N	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
5	O	61/75 (81%)	61 (100%)	0	0	100	100
5	P	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
5	Q	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
5	R	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	S	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
6	T	238/290 (82%)	223 (94%)	15 (6%)	0	100	100
6	W	288/290 (99%)	270 (94%)	17 (6%)	1 (0%)	36	71
7	U	288/306 (94%)	269 (93%)	19 (7%)	0	100	100
7	V	282/306 (92%)	265 (94%)	17 (6%)	0	100	100
7	X	291/306 (95%)	278 (96%)	13 (4%)	0	100	100
7	Y	279/306 (91%)	267 (96%)	11 (4%)	1 (0%)	30	66
8	Z	282/1048 (27%)	270 (96%)	12 (4%)	0	100	100
All	All	10968/17882 (61%)	10400 (95%)	558 (5%)	10 (0%)	49	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	266	GLY
4	L	266	GLY
4	M	266	GLY

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Mol	Chain	Res	Type
4	M	764	GLU
7	Y	297	ASN

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	39/1941 (2%)	39 (100%)	0	100	100
1	C	38/1941 (2%)	38 (100%)	0	100	100
2	E	75/526 (14%)	75 (100%)	0	100	100
2	F	77/526 (15%)	77 (100%)	0	100	100
3	G	398/500 (80%)	398 (100%)	0	100	100
4	H	1142/1192 (96%)	1142 (100%)	0	100	100
4	I	1175/1192 (99%)	1175 (100%)	0	100	100
4	J	1146/1192 (96%)	1146 (100%)	0	100	100
4	K	1129/1192 (95%)	1129 (100%)	0	100	100
4	L	1175/1192 (99%)	1175 (100%)	0	100	100
4	M	1175/1192 (99%)	1175 (100%)	0	100	100
5	N	59/68 (87%)	59 (100%)	0	100	100
5	O	59/68 (87%)	59 (100%)	0	100	100
5	P	59/68 (87%)	59 (100%)	0	100	100
5	Q	59/68 (87%)	58 (98%)	1 (2%)	53	67
5	R	59/68 (87%)	59 (100%)	0	100	100
5	S	59/68 (87%)	59 (100%)	0	100	100
6	T	211/252 (84%)	211 (100%)	0	100	100
6	W	252/252 (100%)	252 (100%)	0	100	100
7	U	262/273 (96%)	262 (100%)	0	100	100
7	V	260/273 (95%)	260 (100%)	0	100	100
7	X	263/273 (96%)	263 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Y	257/273 (94%)	257 (100%)	0	100	100
8	Z	255/883 (29%)	255 (100%)	0	100	100
All	All	9683/15473 (63%)	9682 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	Q	37	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	81	HIS
4	L	749	HIS
7	X	45	GLN
4	K	319	HIS
4	K	901	HIS

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.

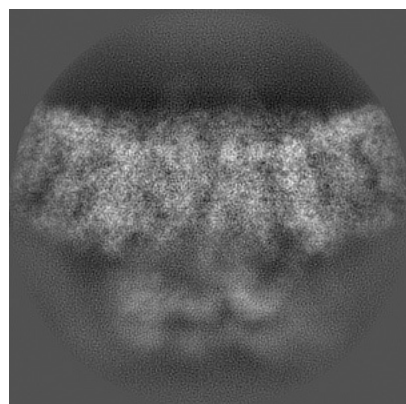
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41201. These allow visual inspection of the internal detail of the map and identification of artifacts.

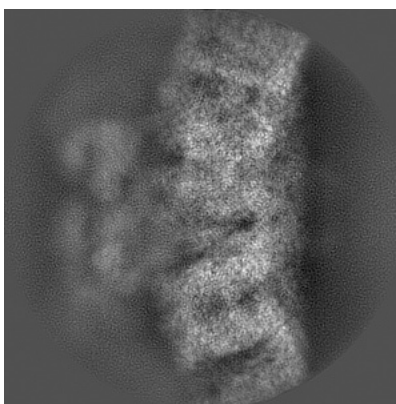
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

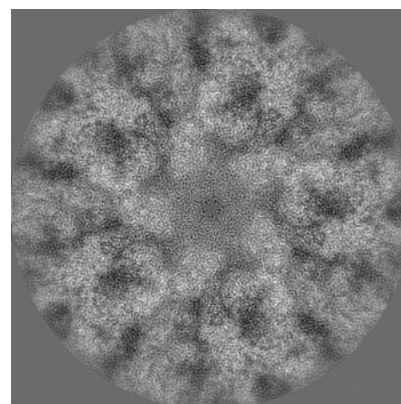
6.1.1 Primary map



X

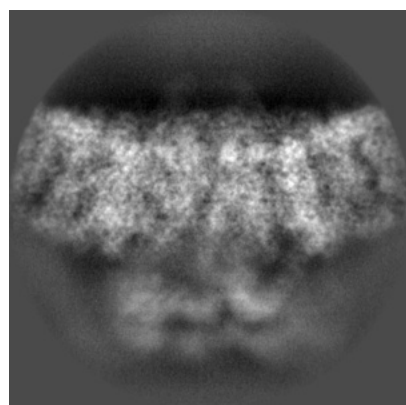


Y

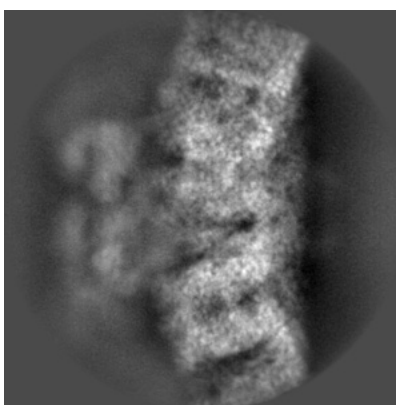


Z

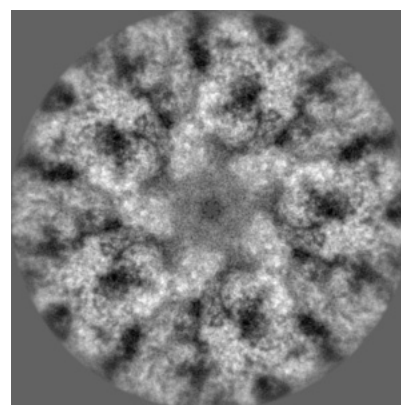
6.1.2 Raw map



X



Y

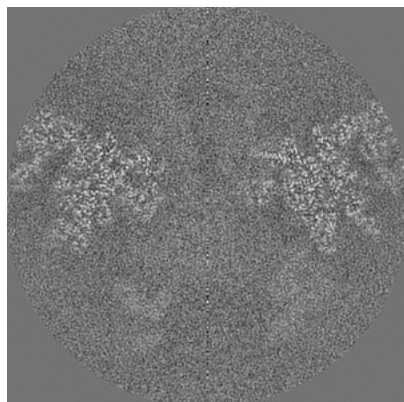


Z

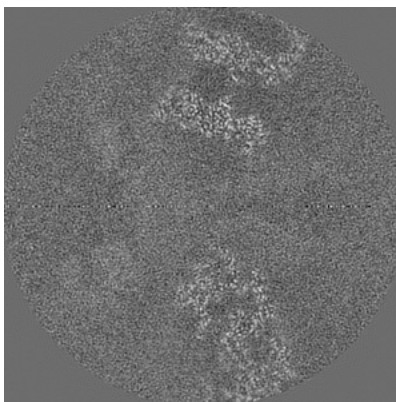
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

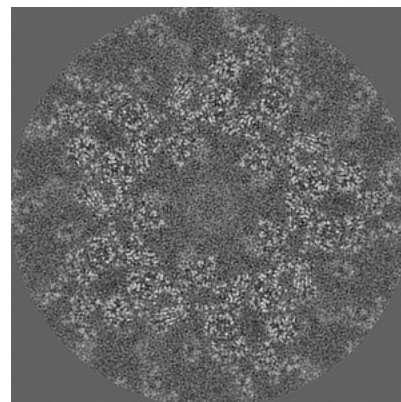
6.2.1 Primary map



X Index: 180

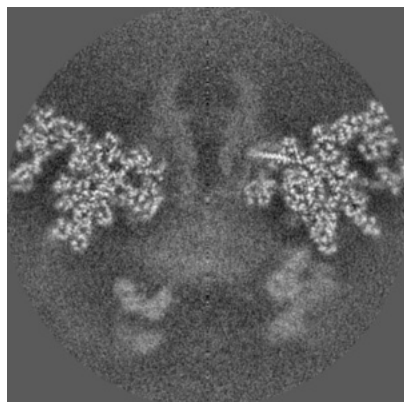


Y Index: 180

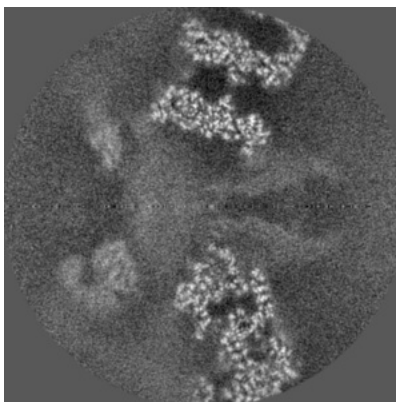


Z Index: 180

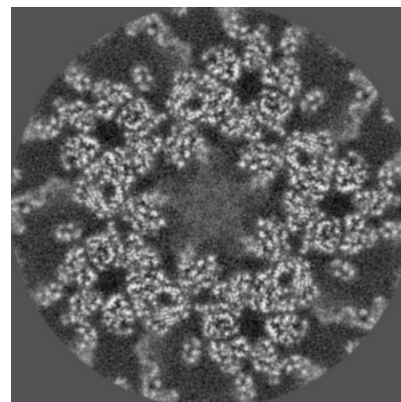
6.2.2 Raw map



X Index: 180



Y Index: 180

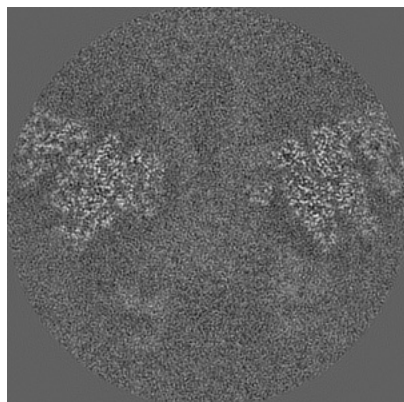


Z Index: 180

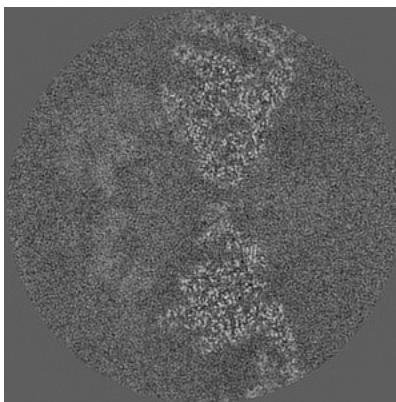
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

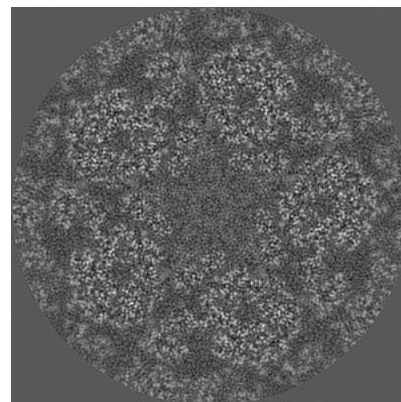
6.3.1 Primary map



X Index: 184

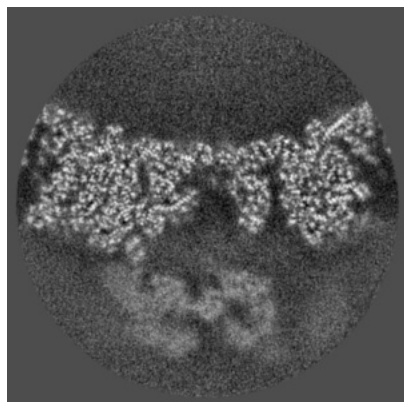


Y Index: 217

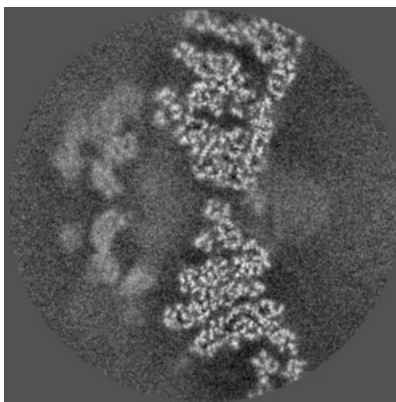


Z Index: 209

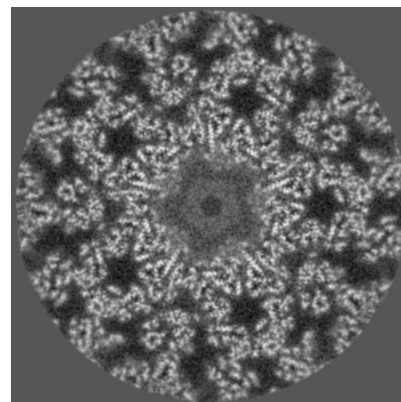
6.3.2 Raw map



X Index: 238



Y Index: 220

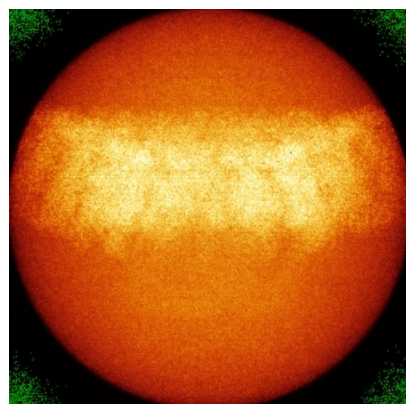


Z Index: 224

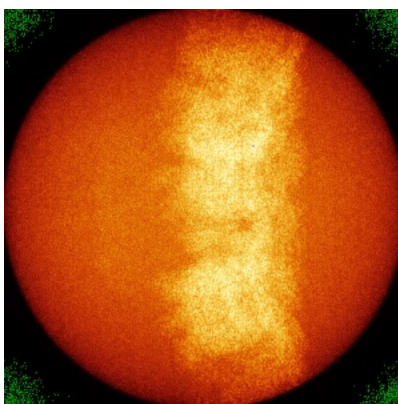
The images above show the largest variance slices of the map in three orthogonal directions.

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

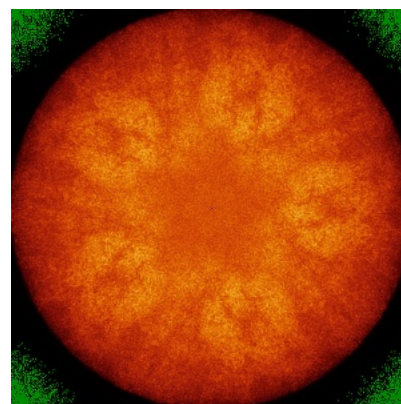
6.4.1 Primary map



X

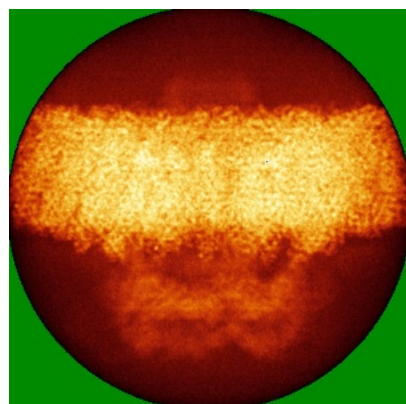


Y

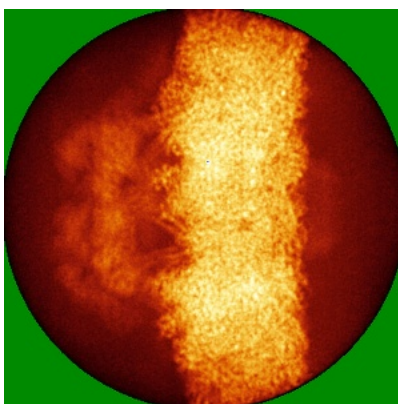


Z

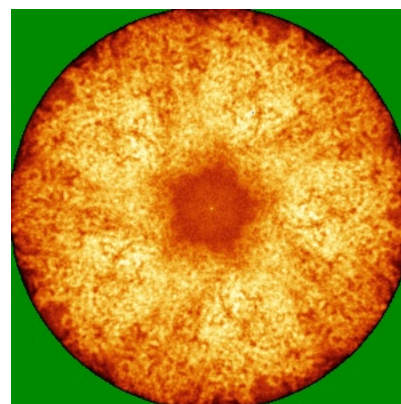
6.4.2 Raw map



X



Y

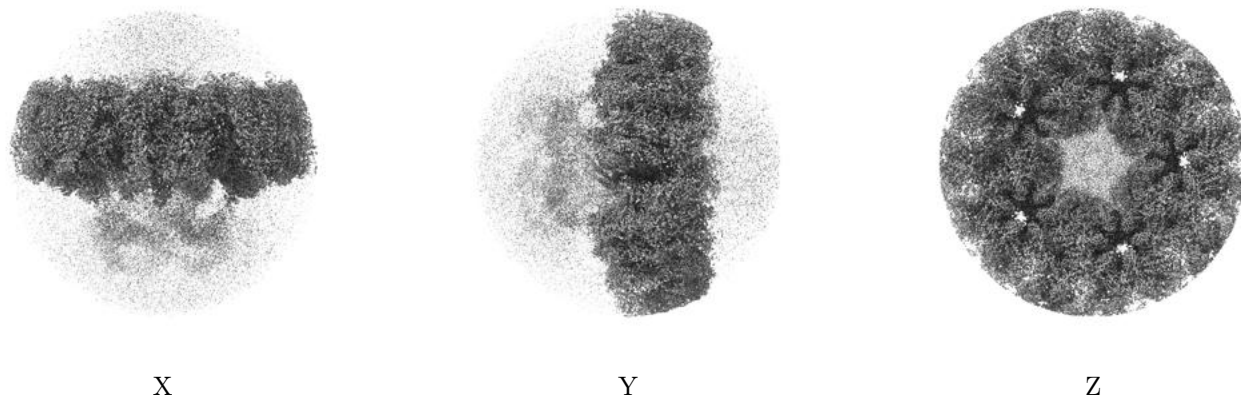


Z

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.

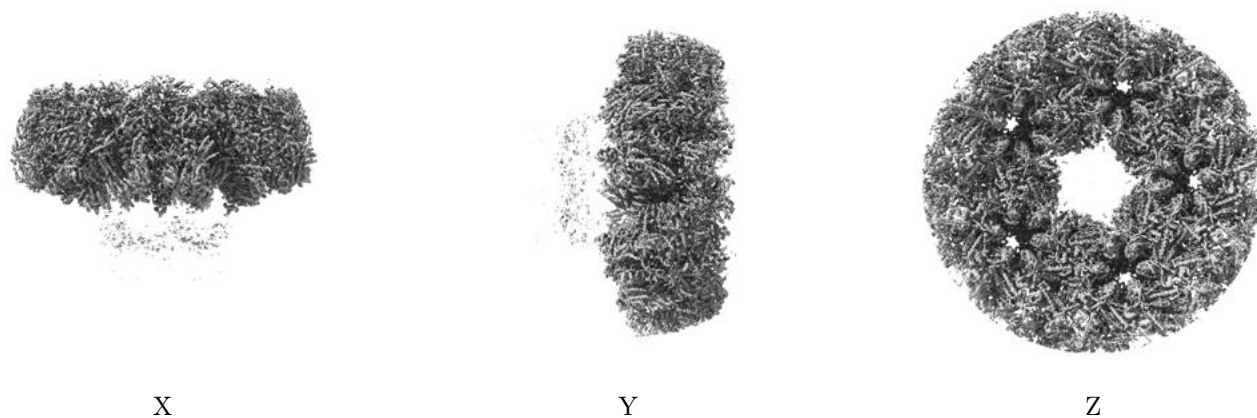
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. 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.

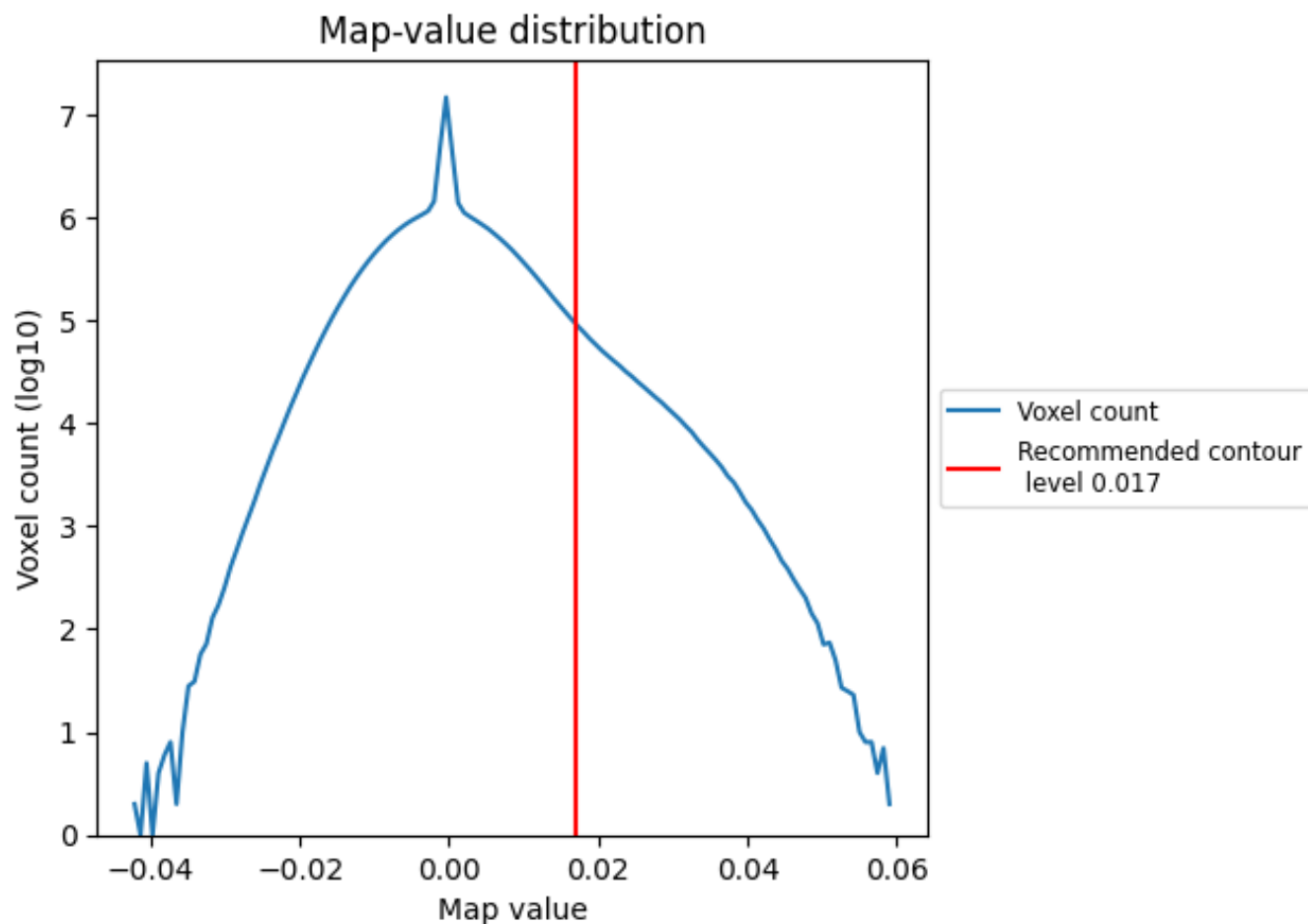
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

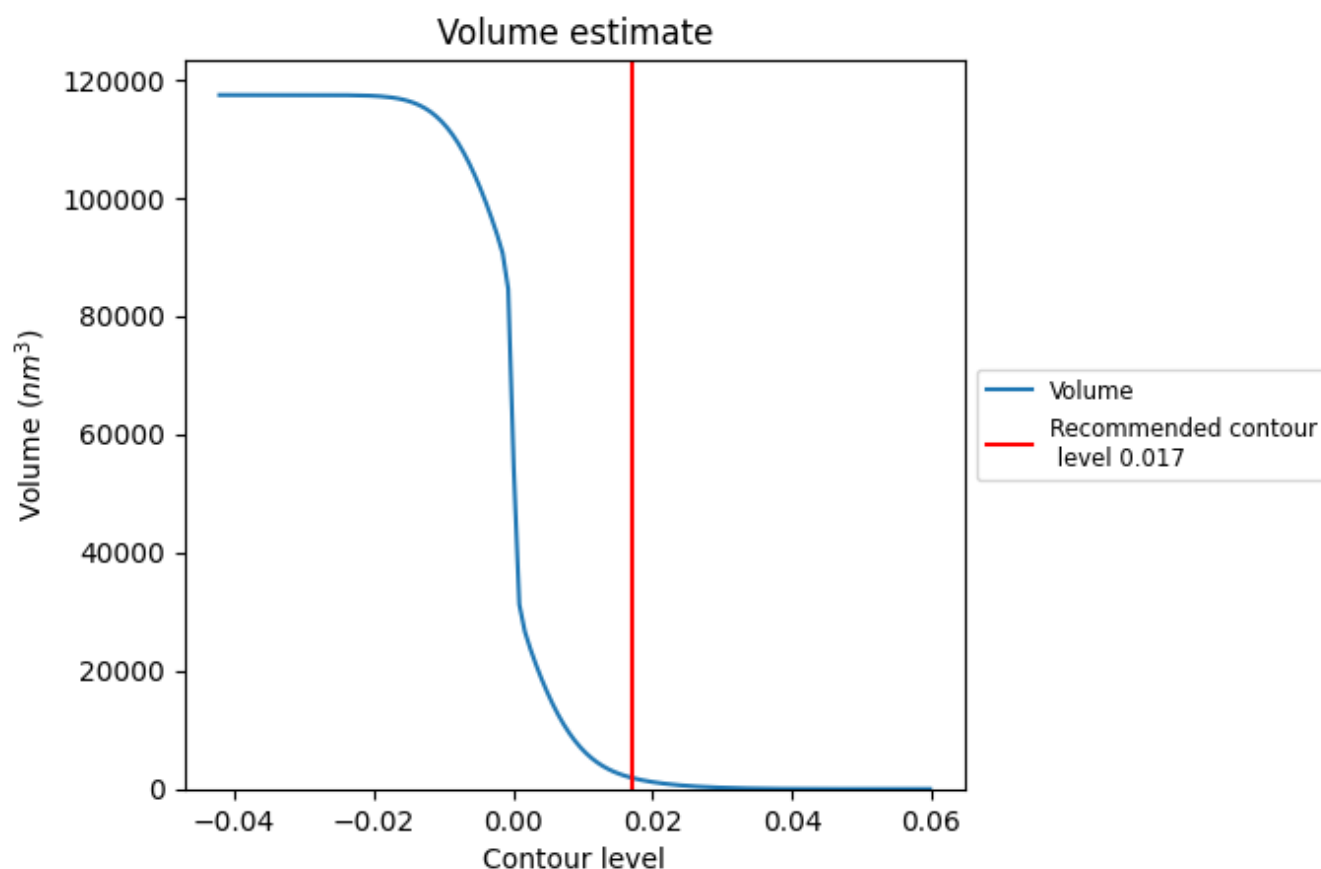
This section contains the results of statistical analysis of the map.

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.

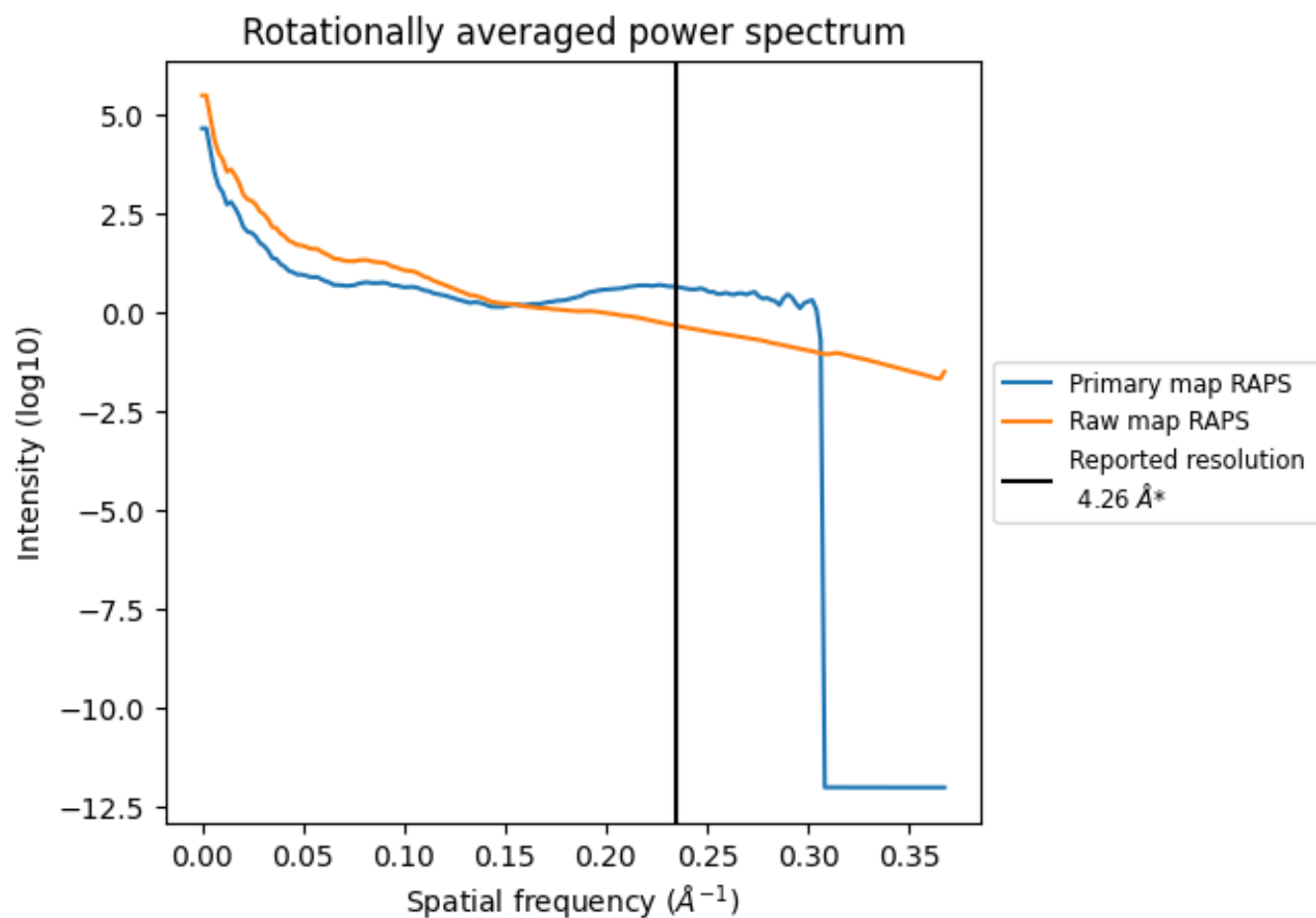
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1898 nm³; this corresponds to an approximate mass of 1714 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 ⓘ

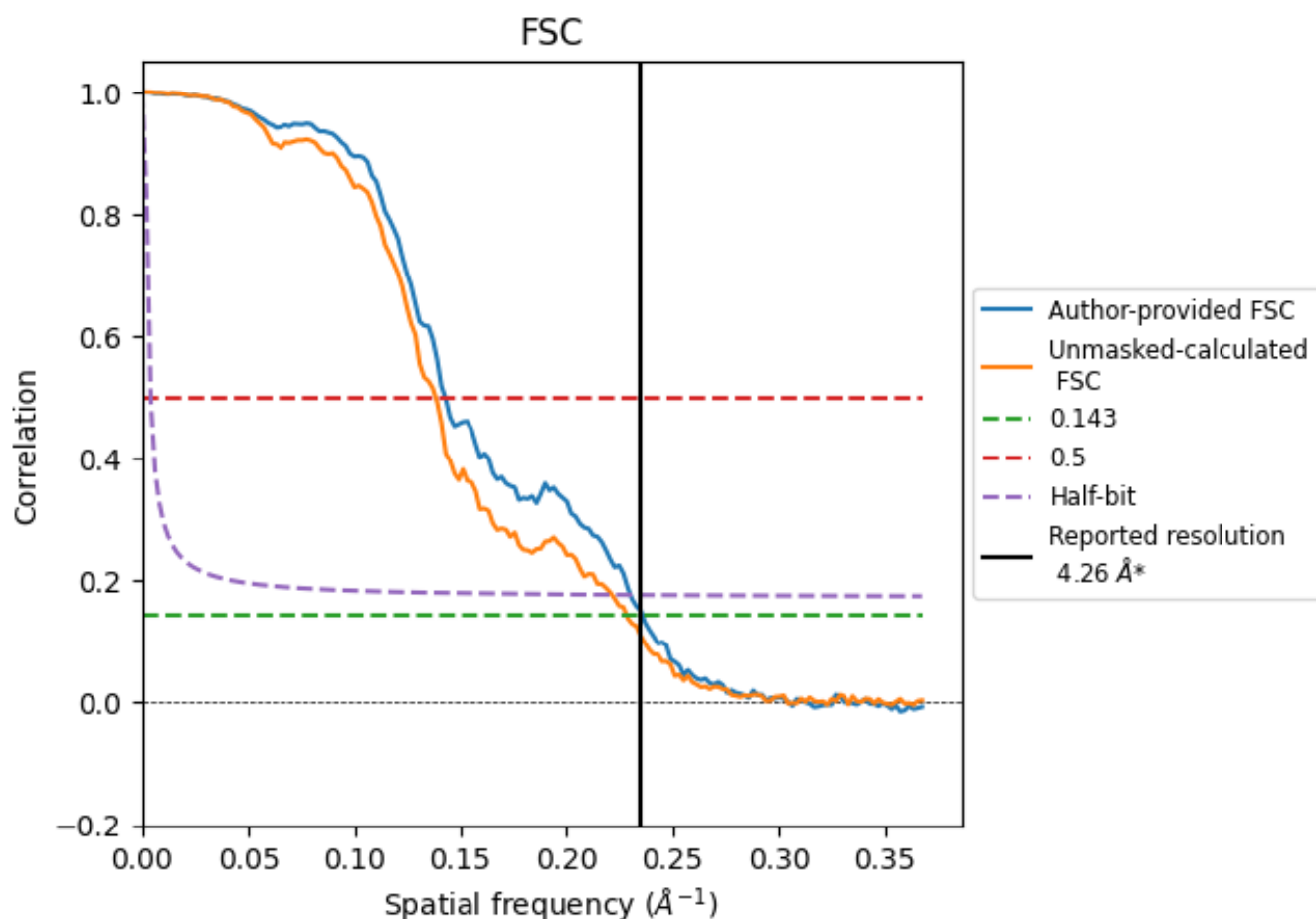


*Reported resolution corresponds to spatial frequency of 0.235 Å⁻¹

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 $0.235 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

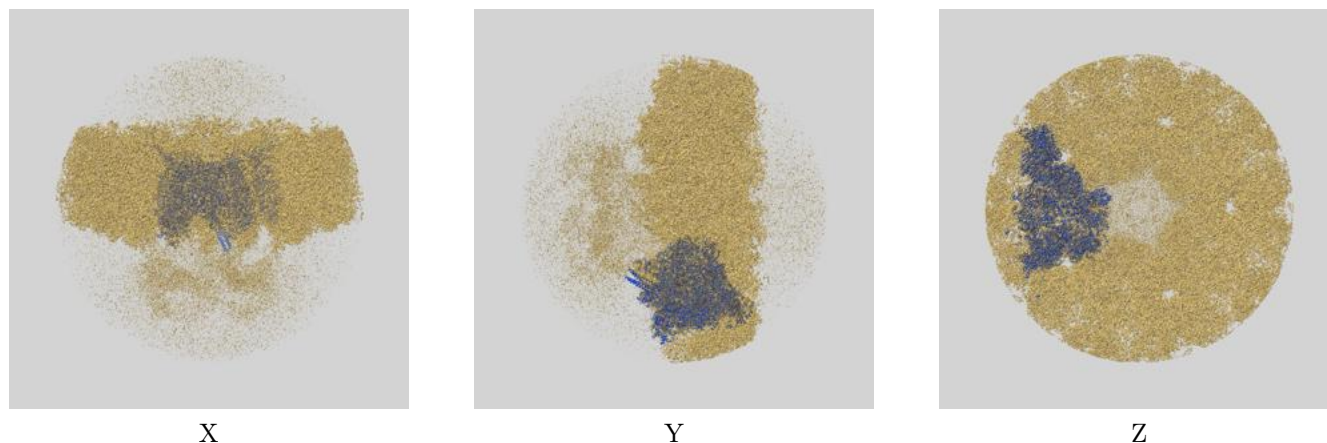
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.26	-	-
Author-provided FSC curve	4.24	7.01	4.35
Unmasked-calculated*	4.38	7.24	4.52

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

9 Map-model fit [i](#)

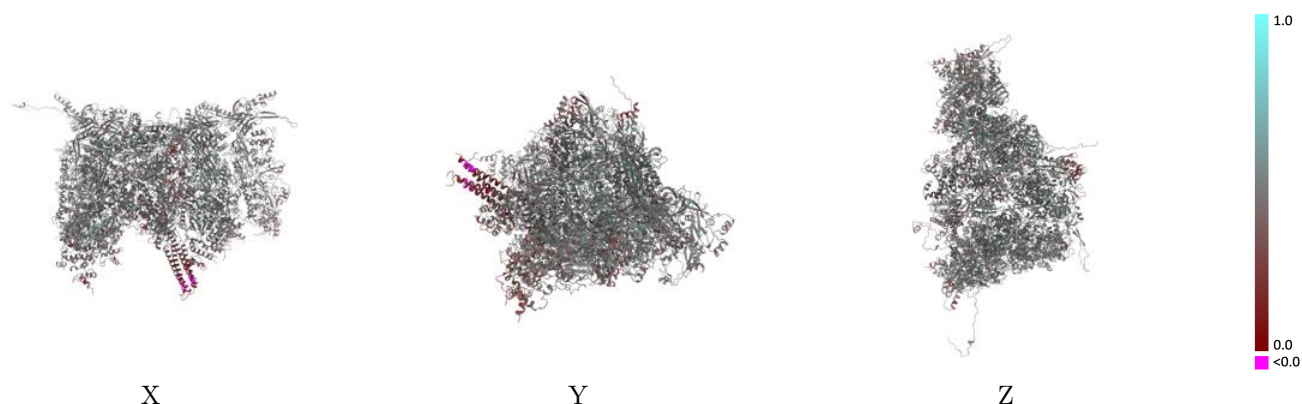
This section contains information regarding the fit between EMDB map EMD-41201 and PDB model 8TET. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



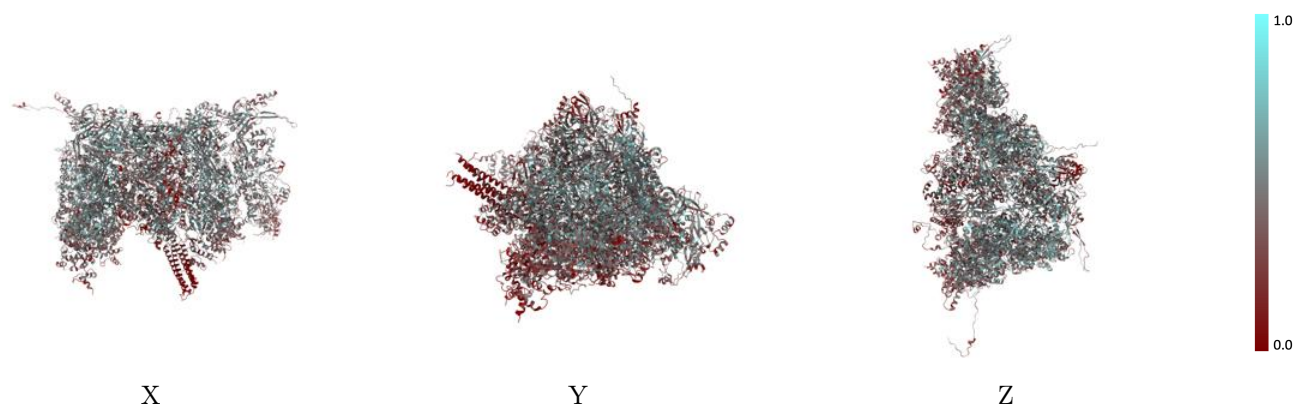
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



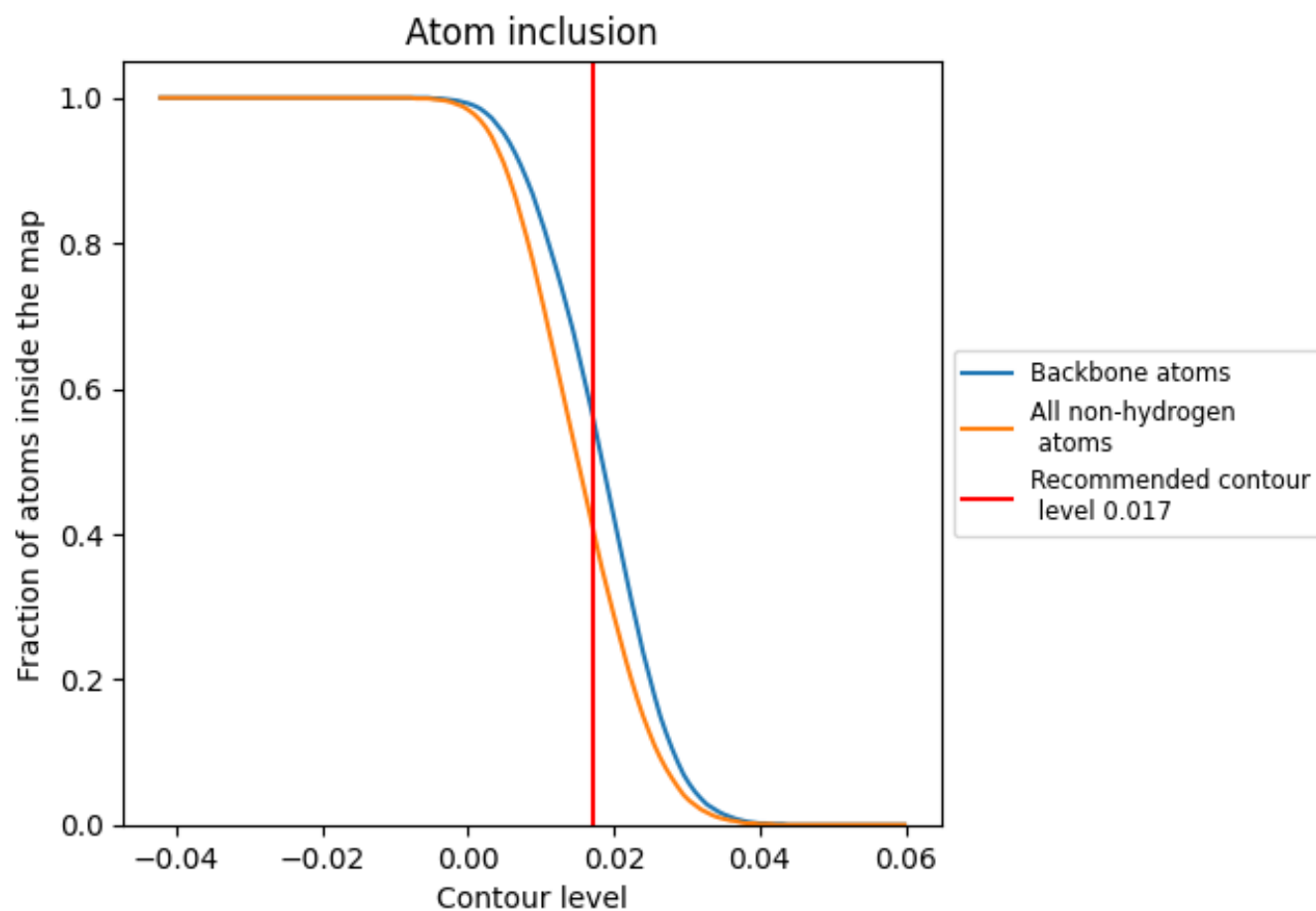
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 41% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4130	 0.4610
A	 0.1300	 0.2550
C	 0.0740	 0.2390
E	 0.2090	 0.3520
F	 0.1210	 0.2820
G	 0.3770	 0.4510
H	 0.4810	 0.4820
I	 0.4830	 0.4830
J	 0.4320	 0.4720
K	 0.4740	 0.4790
L	 0.4490	 0.4760
M	 0.3920	 0.4630
N	 0.2810	 0.3580
O	 0.2610	 0.3920
P	 0.2070	 0.3660
Q	 0.2510	 0.3560
R	 0.1690	 0.3570
S	 0.1590	 0.3540
T	 0.3090	 0.4260
U	 0.3790	 0.4610
V	 0.3810	 0.4560
W	 0.4020	 0.4680
X	 0.3250	 0.4460
Y	 0.3580	 0.4560
Z	 0.2140	 0.4040

