wwPDB EM Validation Summary Report

Nov 10, 2024 – 03:56 AM EST

PDB ID	:	6B43
EMDB ID	:	EMD-7047
Title	:	CryoEM structure and atomic model of the Kaposi's sarcoma-associated herpesvirus capsid
Authors	:	Dai, X.H.; Gong, D.Y.; Sun, R.; Zhou, Z.H.
Deposited on	:	2017-09-25
Resolution	:	4.20 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:

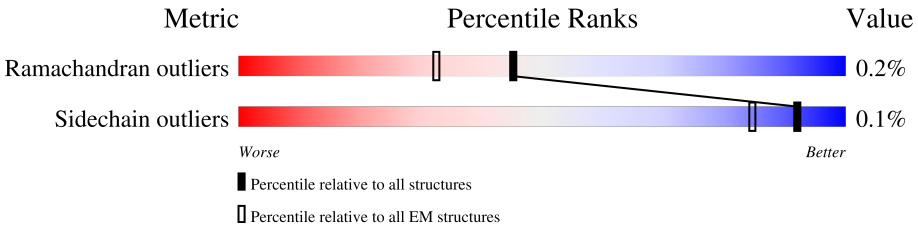
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 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 <=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	4	1376	58% 87% · 12%
1	A	1376	9% 98% ··
1	B	1376	10% 98% ··
1	C	1376	11% 97% ··
1	D	1376	11% 97% ··
1	E	1376	10% 98% ··
1	F	1376	10% 97% ··
1	M	1376	9% 98% ··
1	N	1376	9% 98% ··

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Mol	Chain	Length	Quality of chain
1	O	1376	9% 97%
1	S	1376	19% 92% 7%
1	T	1376	14% 98%
1	U	1376	12% 98%
1	V	1376	13% 97%
1	W	1376	16% 98%
1	X	1376	20% 97%
2	0	170	22% 46% 54%
2	1	170	20% 46% 54%
2	2	170	28% 46% 54%
2	3	170	29% 46% 54%
2	G	170	16% 46% 54%
2	H	170	26% 46% 54%
2	I	170	14% 46% 54%
2	J	170	18% 46% 54%
2	K	170	15% 46% 54%
2	L	170	13% 46% 54%
2	P	170	15% 46% 54%
2	Q	170	20% 46% 54%
2	R	170	15% 46% 54%
2	Y	170	28% 46% 54%
2	Z	170	31% 46% 54%
3	5	331	59% 95%
3	8	331	11% 97%
3	b	331	12% 97%

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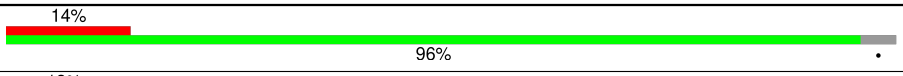
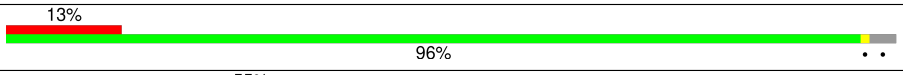
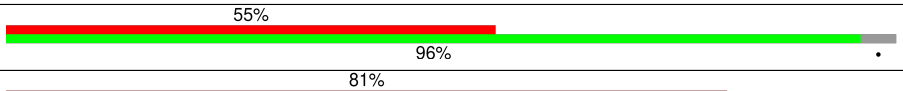
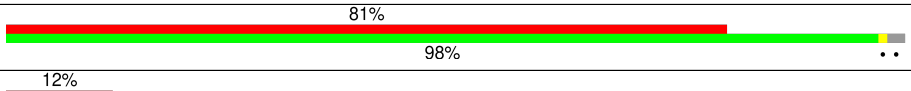
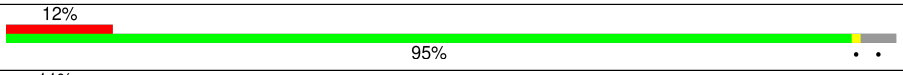
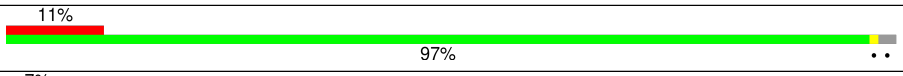
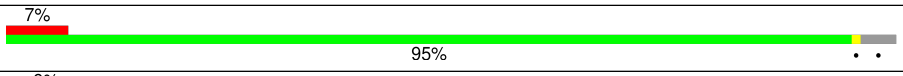
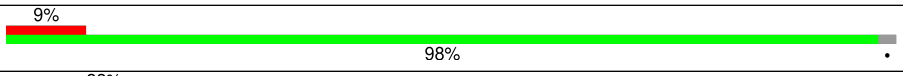
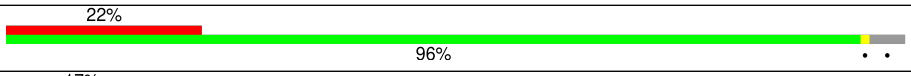
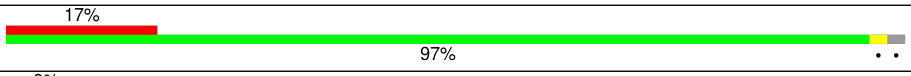
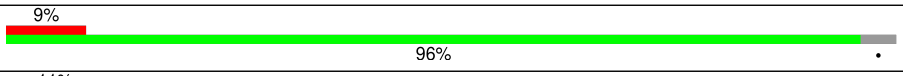
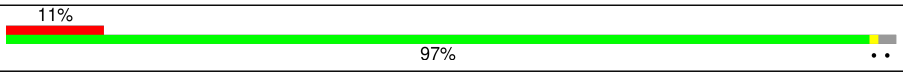
Mol	Chain	Length	Quality of chain
3	e	331	
3	h	331	
4	6	305	
4	7	305	
4	9	305	
4	a	305	
4	c	305	
4	d	305	
4	f	305	
4	g	305	
4	i	305	
4	j	305	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 214334 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	B	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	C	1354	Total	C	N	O	S	0	0
			10621	6748	1842	1959	72		
1	D	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	E	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	F	1356	Total	C	N	O	S	0	0
			10638	6757	1847	1961	73		
1	M	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	N	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	O	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	S	1281	Total	C	N	O	S	0	0
			10060	6397	1737	1855	71		
1	T	1360	Total	C	N	O	S	0	0
			10666	6776	1851	1966	73		
1	U	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	V	1352	Total	C	N	O	S	0	0
			10604	6739	1839	1954	72		
1	W	1354	Total	C	N	O	S	0	0
			10621	6748	1842	1959	72		
1	X	1345	Total	C	N	O	S	0	0
			10548	6701	1829	1946	72		
1	4	1216	Total	C	N	O	S	0	0
			9586	6102	1665	1748	71		

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	H	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	I	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	J	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	K	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	L	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	P	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Q	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	R	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Y	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Z	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	0	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	1	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	2	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	3	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	319	Total	C	N	O	S	0	0
			2463	1578	421	449	15		
3	8	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		
3	b	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		
3	e	319	Total	C	N	O	S	0	0
			2460	1575	422	448	15		
3	h	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		

- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	7	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	9	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	a	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	c	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	d	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	f	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	g	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	i	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	j	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		

3 Residue-property plots (i)

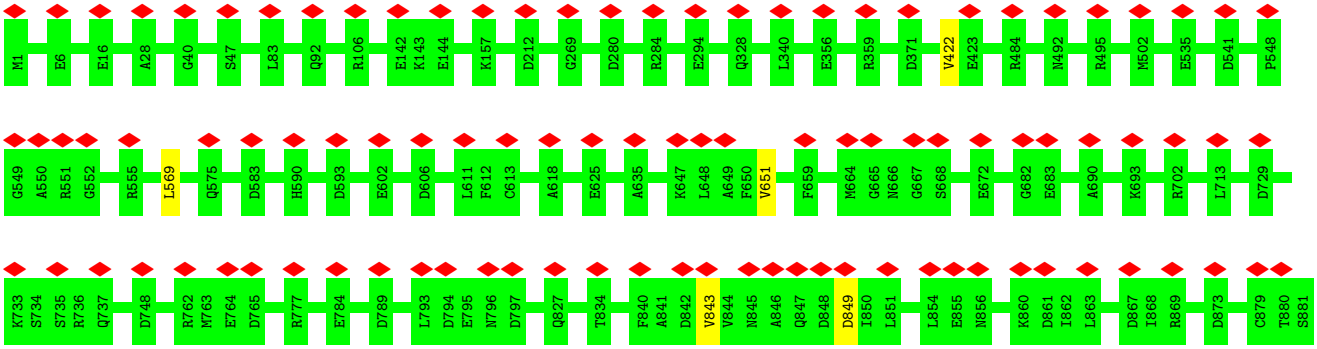
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

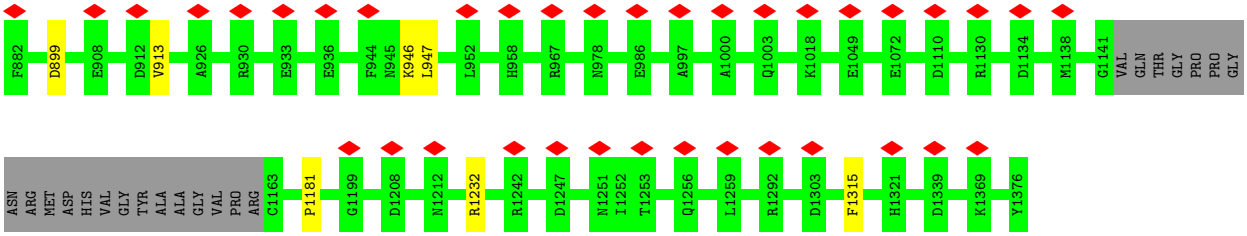
• Molecule 1: Major capsid protein

Chain A:

• Molecule 1: Major capsid protein

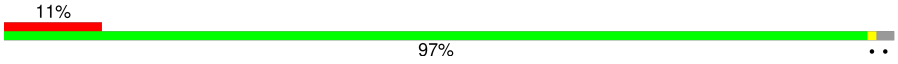
Chain B:

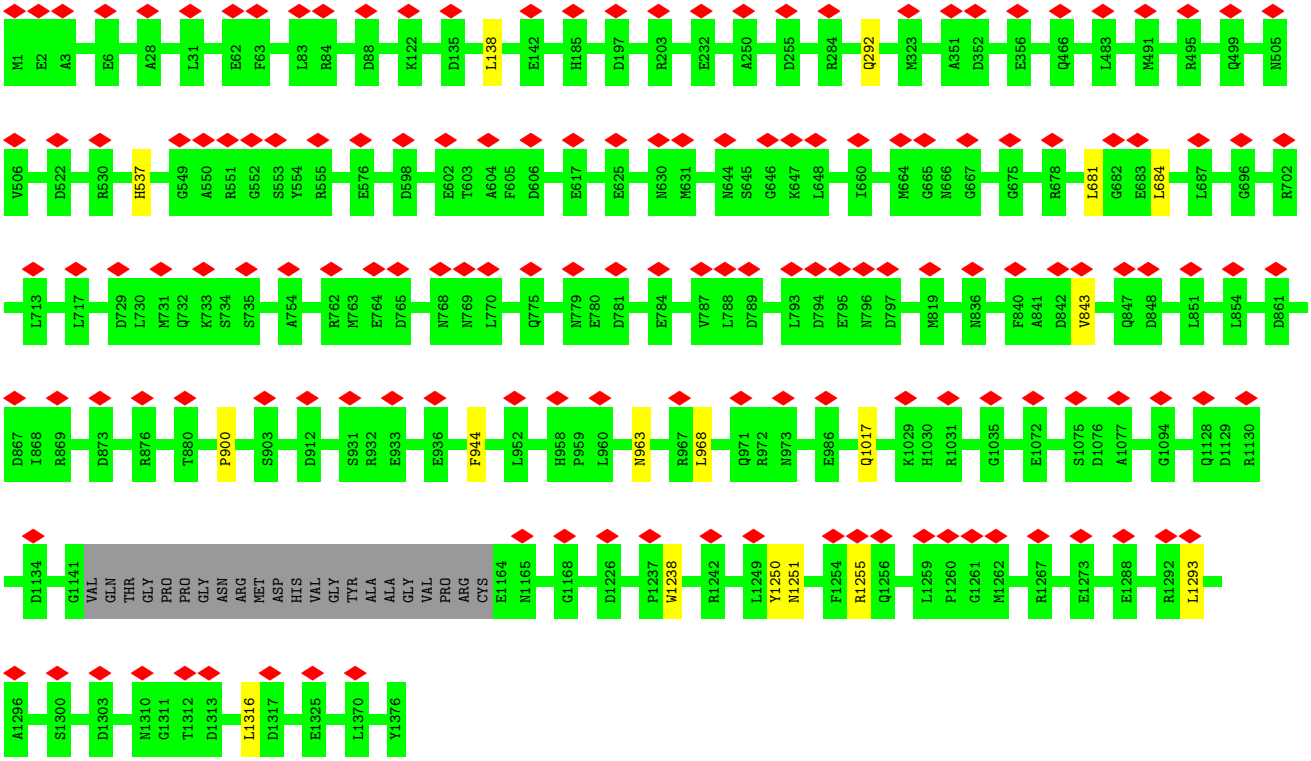




• Molecule 1: Major capsid protein

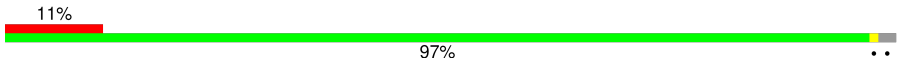
Chain C:

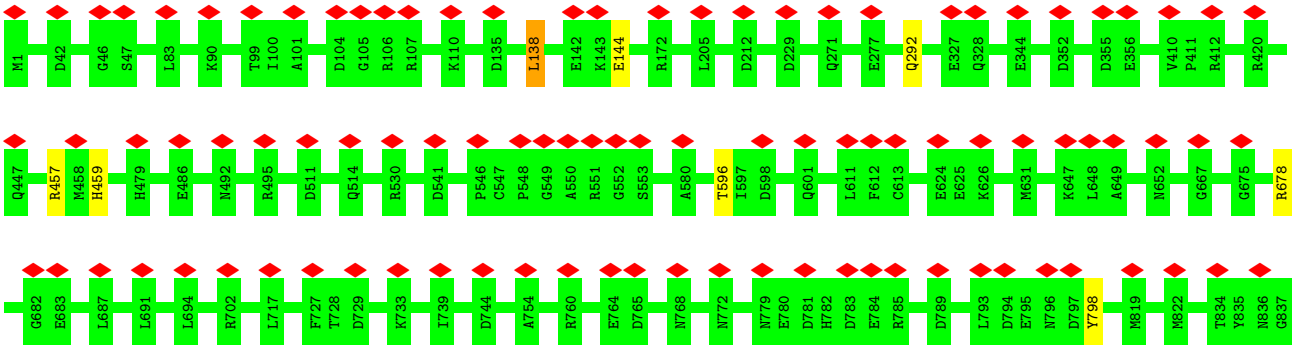


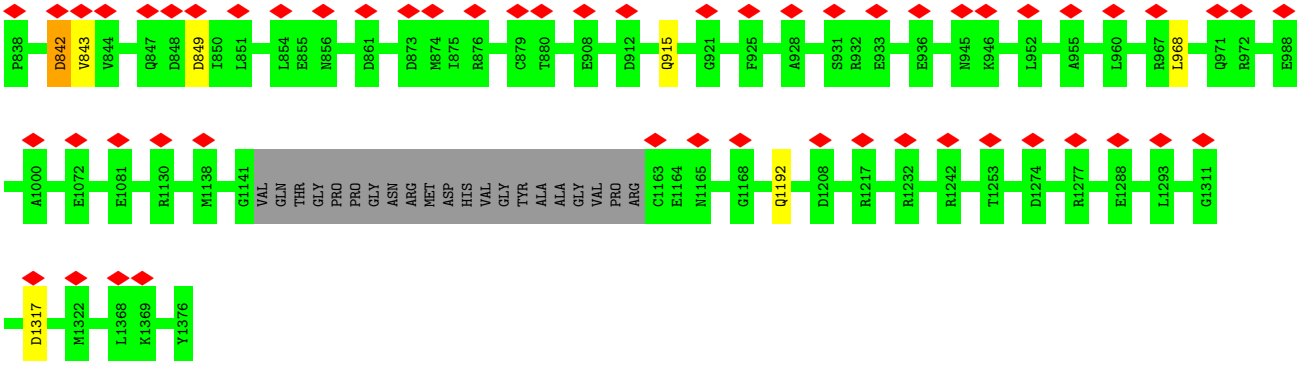


• Molecule 1: Major capsid protein

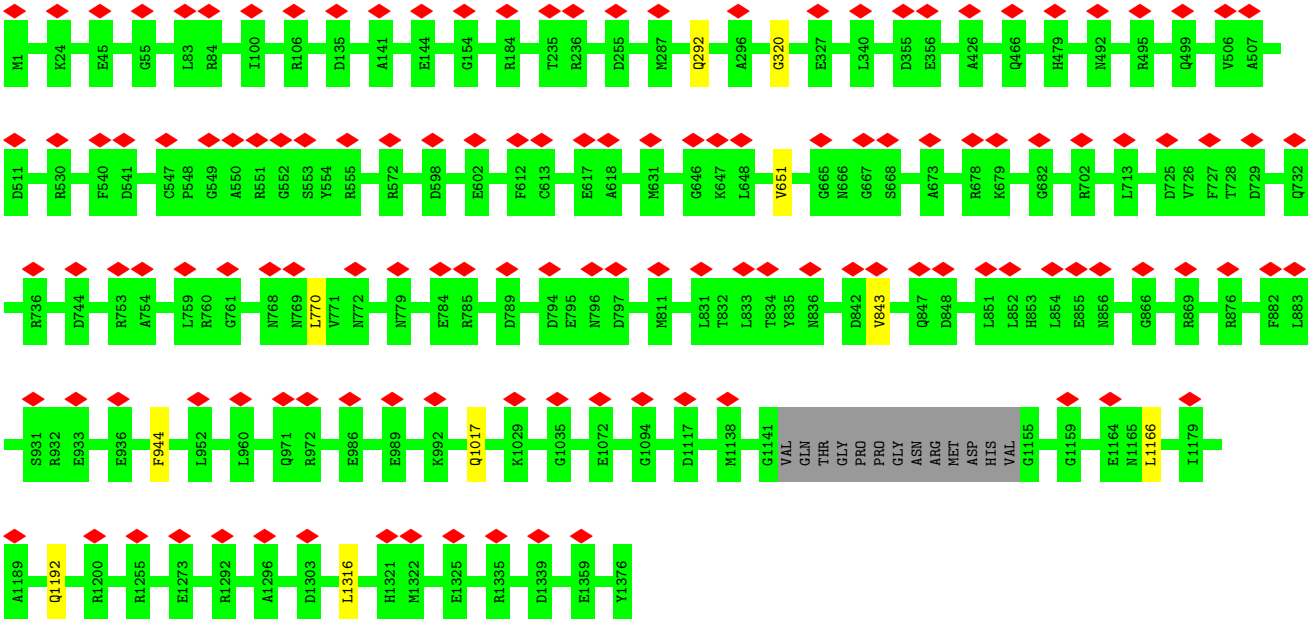
Chain D:



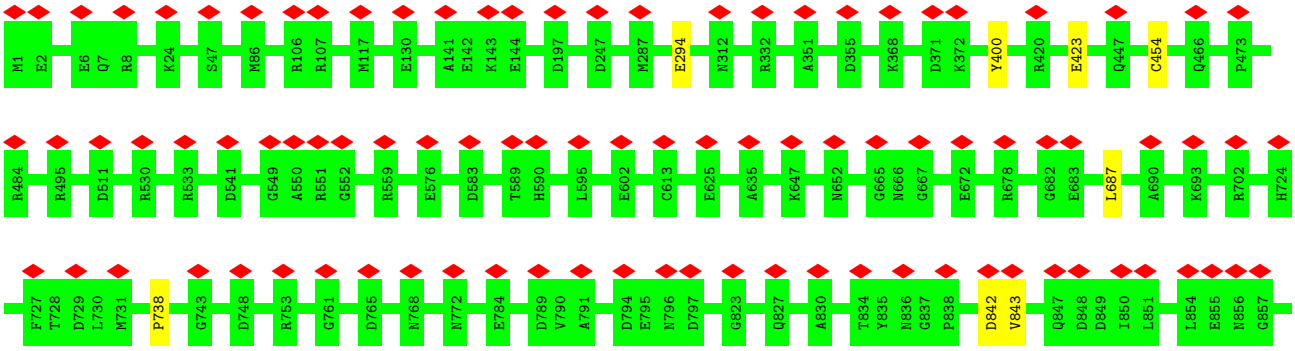


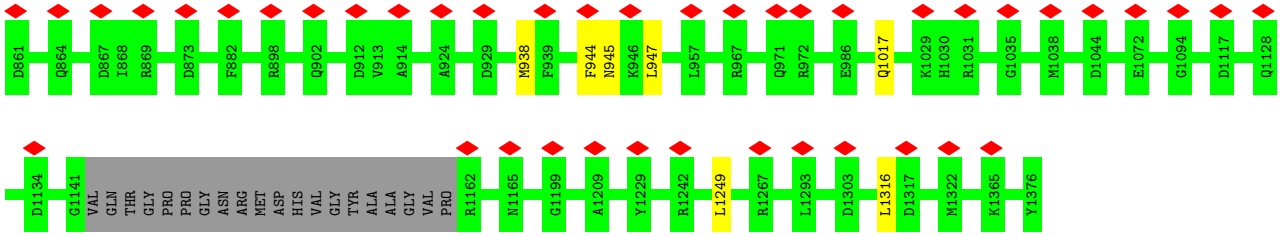


• Molecule 1: Major capsid protein



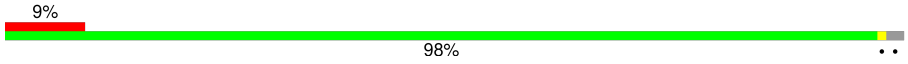
• Molecule 1: Major capsid protein





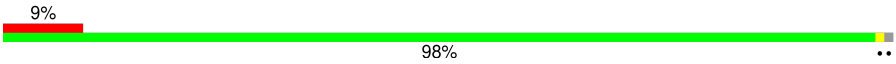
• Molecule 1: Major capsid protein

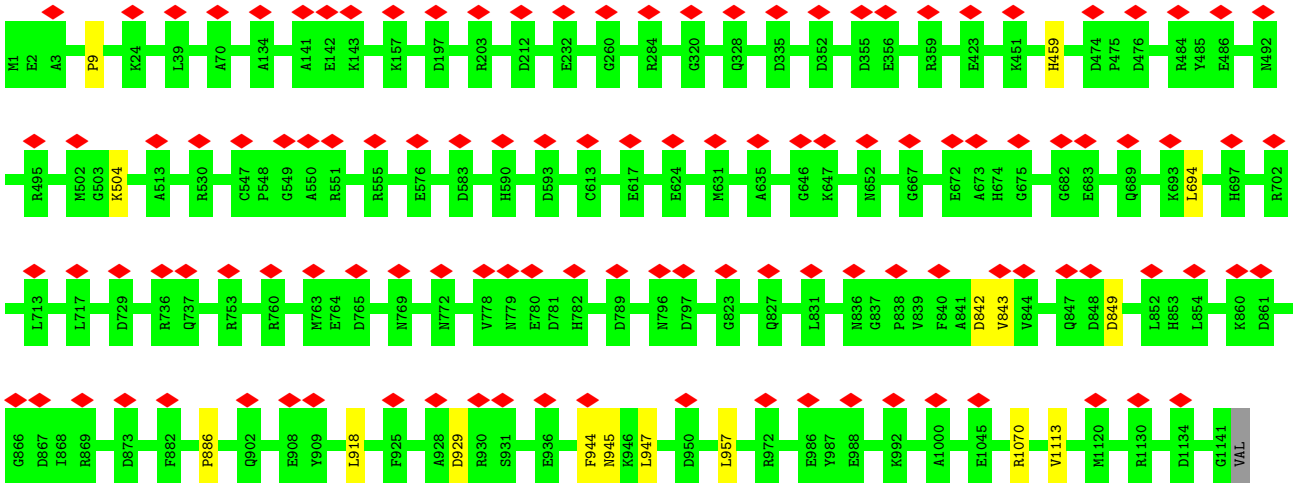
Chain M:

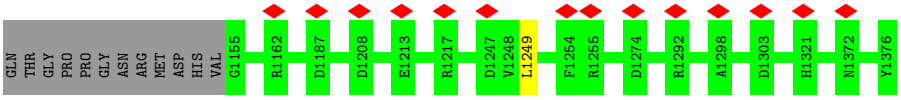


• Molecule 1: Major capsid protein

Chain N:

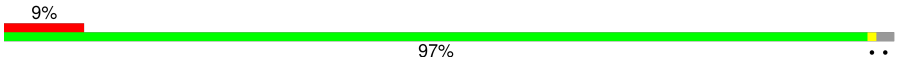


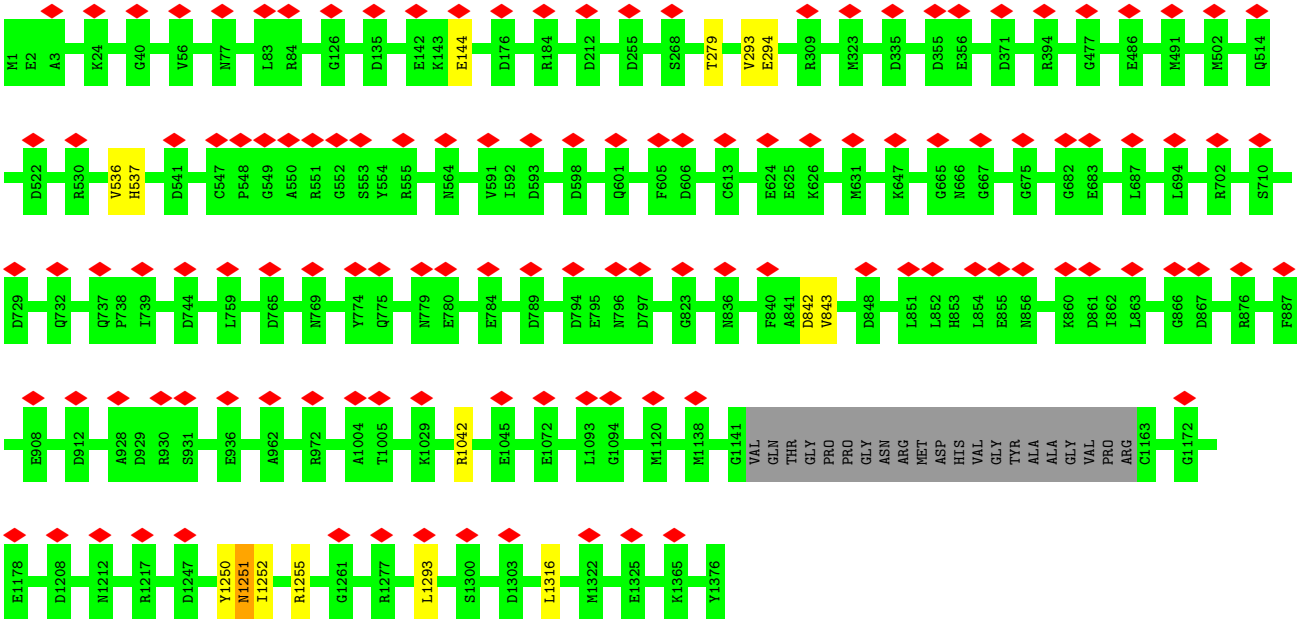




• Molecule 1: Major capsid protein

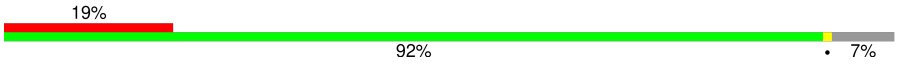
Chain O:

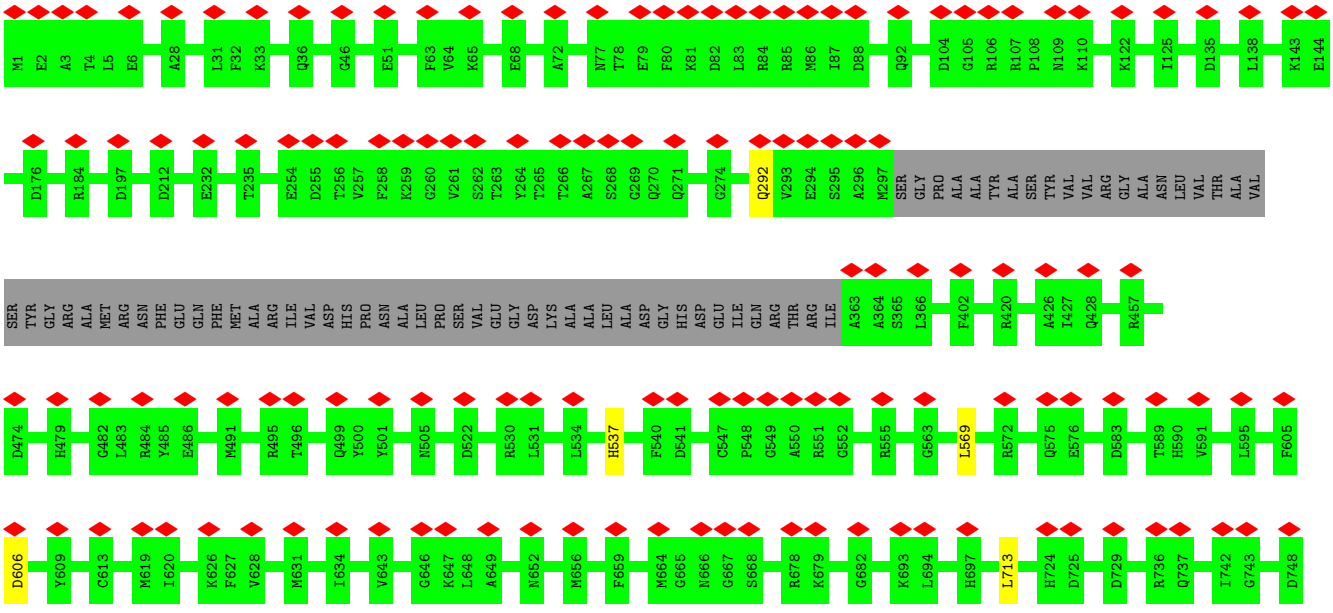


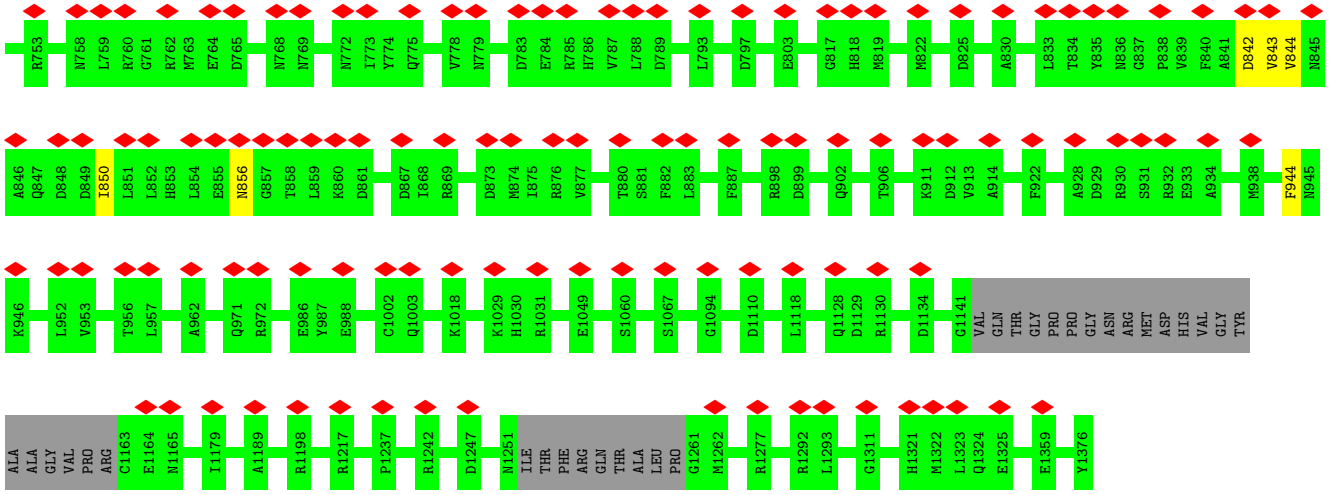


• Molecule 1: Major capsid protein

Chain S:

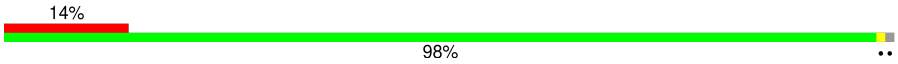


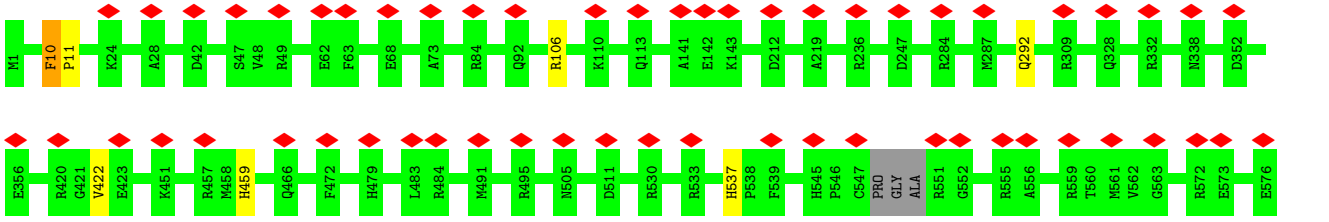




• Molecule 1: Major capsid protein

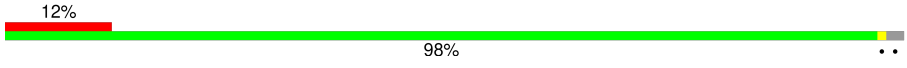
Chain T:





• Molecule 1: Major capsid protein

Chain U:

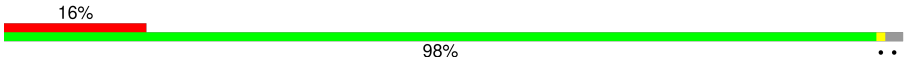


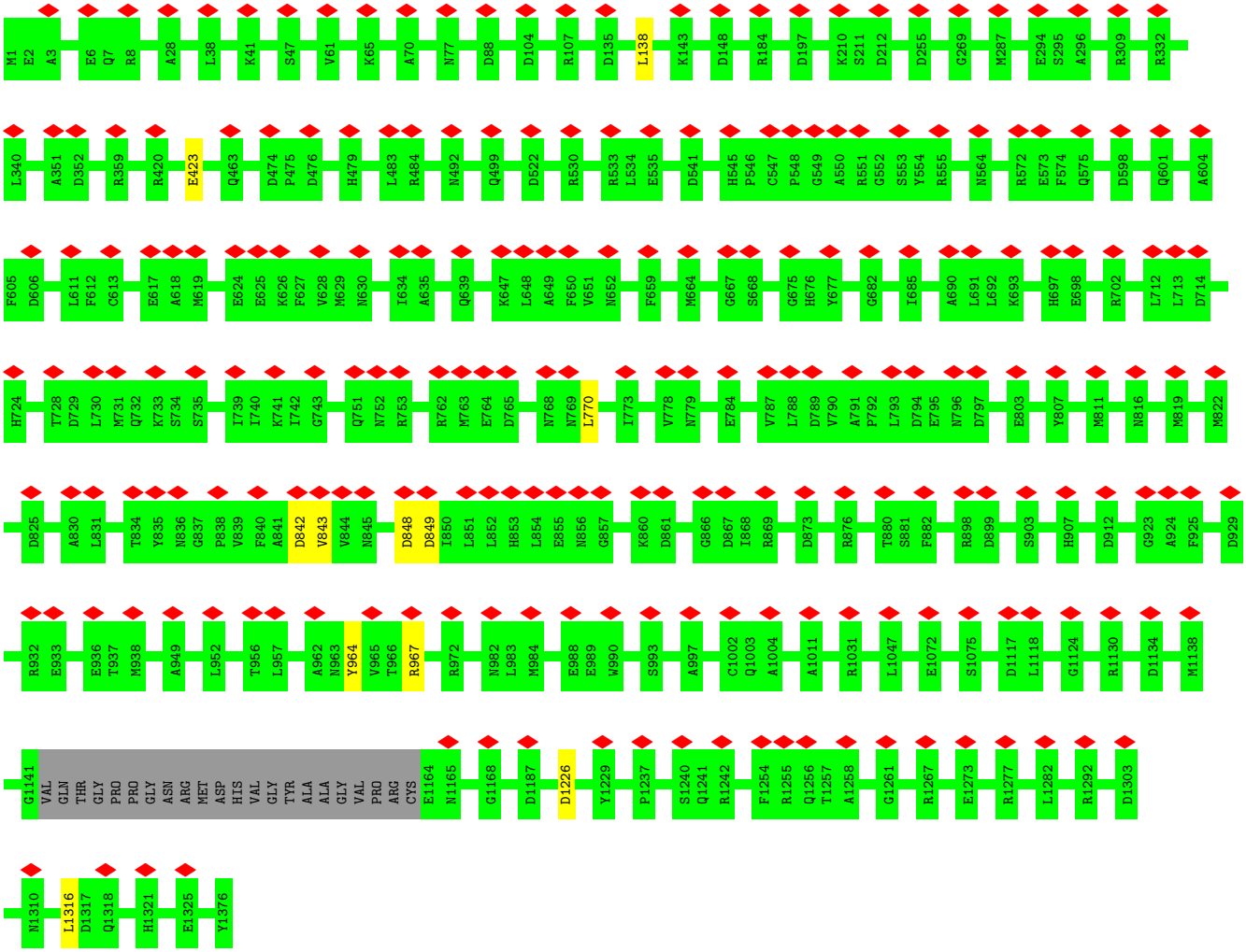
• Molecule 1: Major capsid protein

Chain V:

• Molecule 1: Major capsid protein

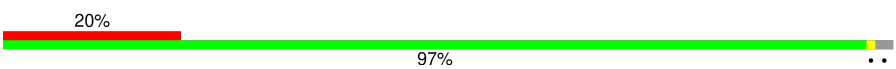
Chain W:

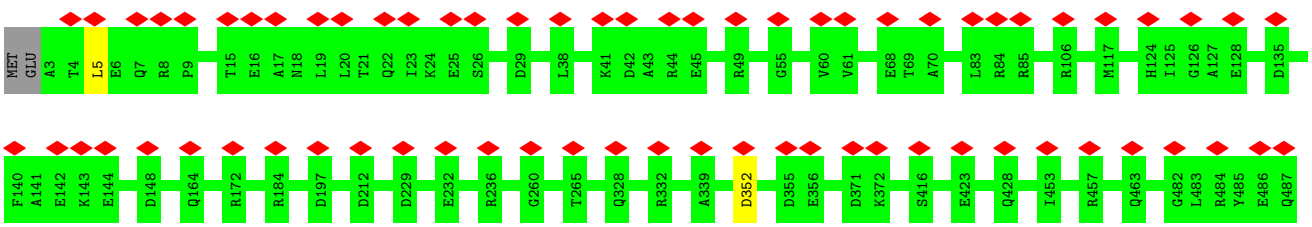


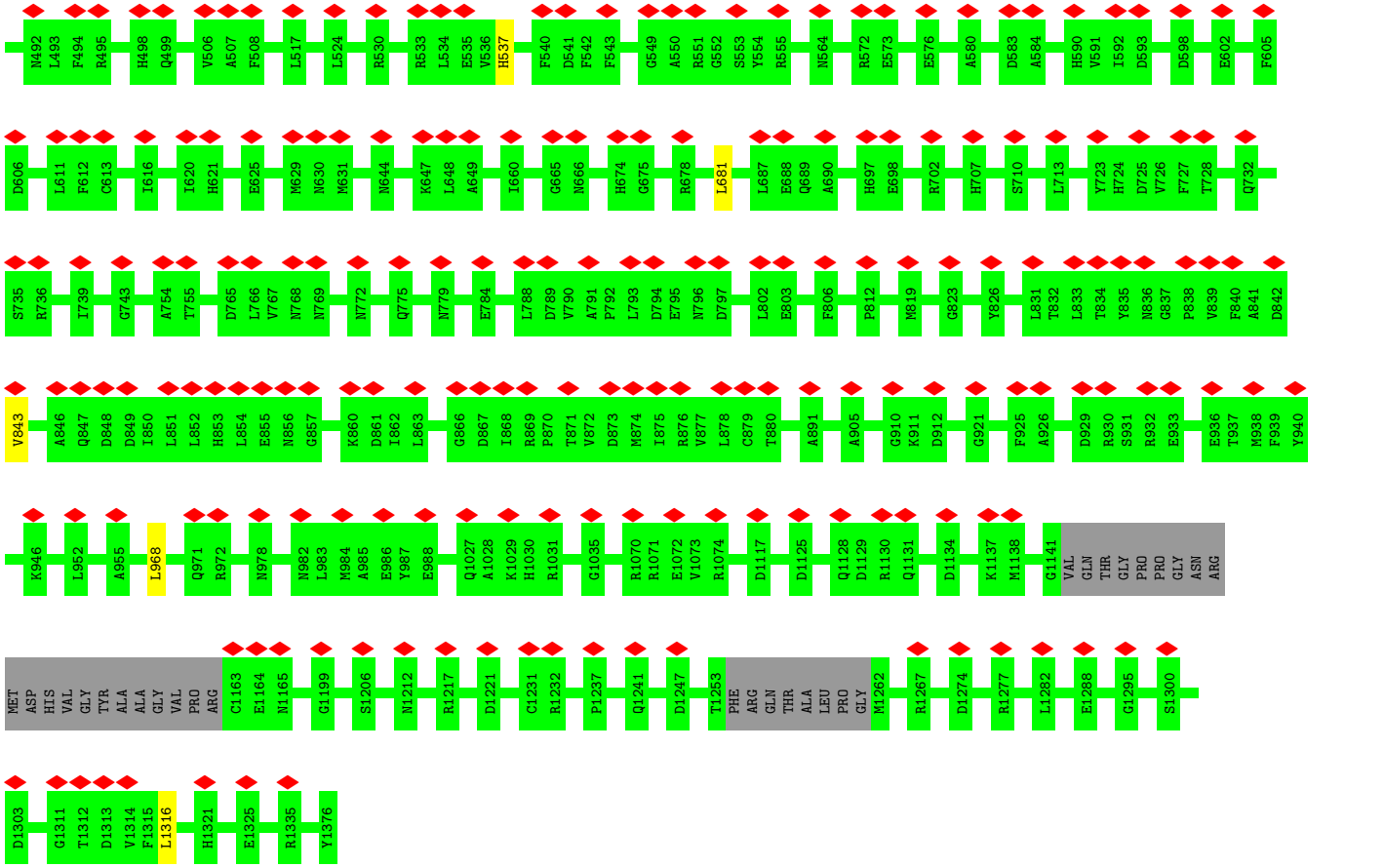


• Molecule 1: Major capsid protein

Chain X:

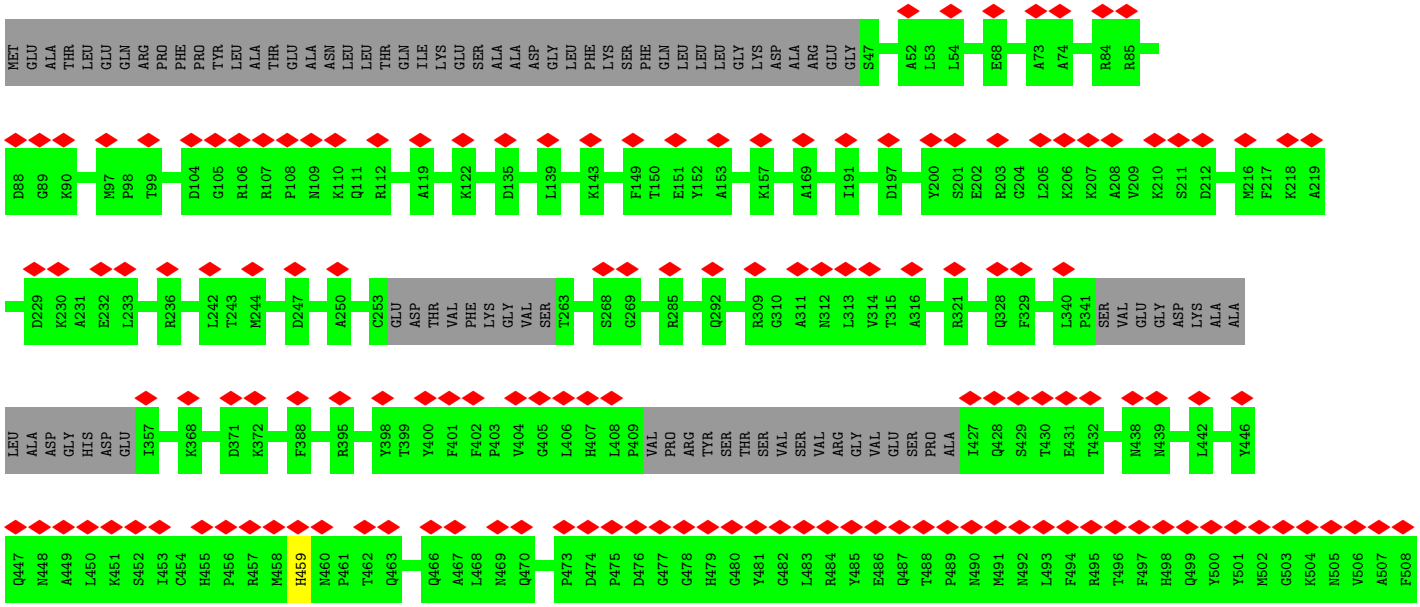


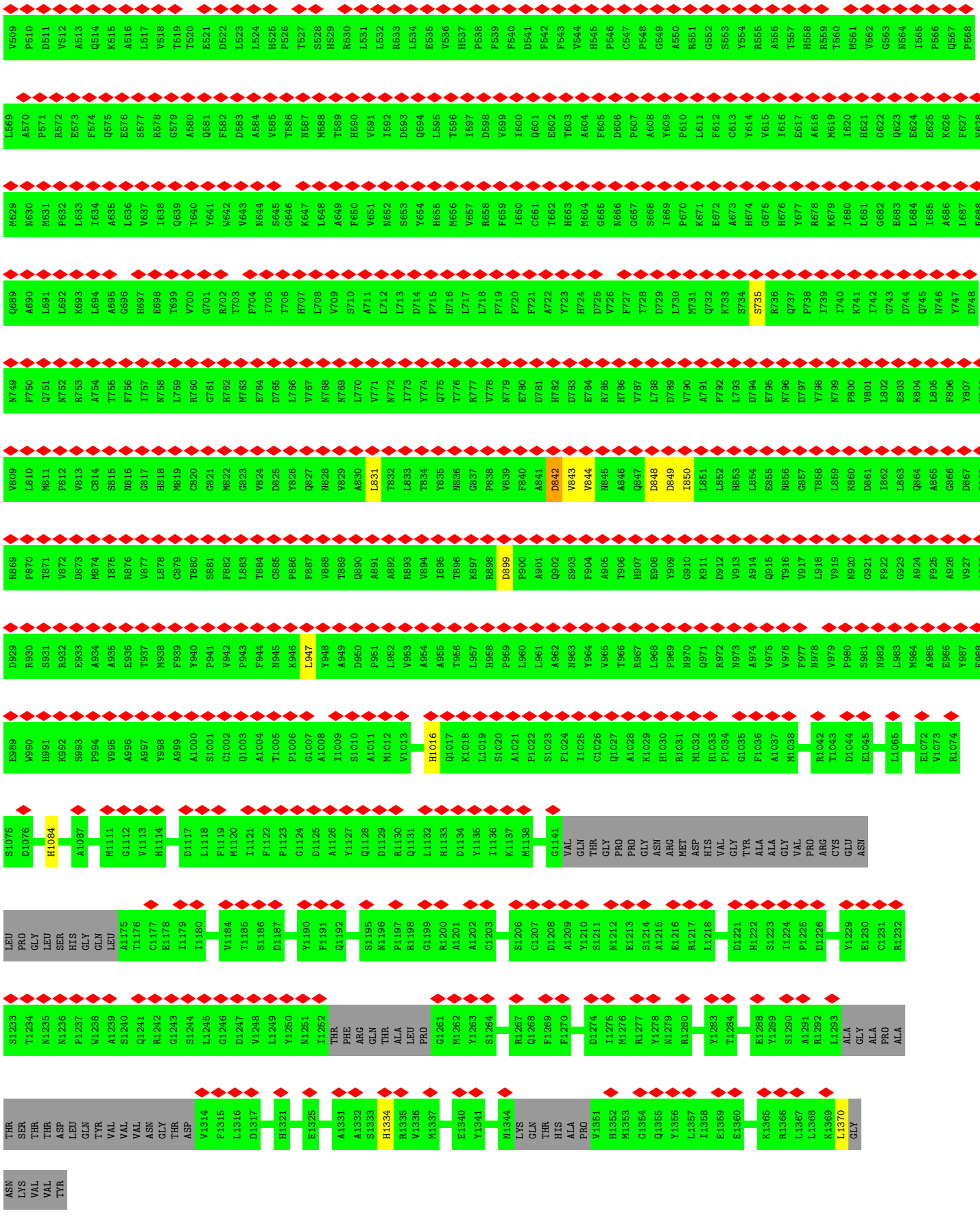




• Molecule 1: Major capsid protein

Chain 4:

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LEU PRO GLY LEU SER HIS GLY GLN LEU A1175 T1176 C1177 E1178 I1179 I1180 V1184 T1185 S1186 D1187 Y1190 F1191 Q1192 S1195 N1196 P1197 R1198 G1199 R1200 A1201 A1202 C1203 S1206 C1207 D1208 A1209 Y1210 S1211 N1212 E1213 S1214 A1215 E1216 R1217 L1218 D1221 H1222 S1223 I1224 P1225 D1226 Y1229 E1230 C1231 R1232
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THR SER THR THR ASP LEU GLN TYR VAL VAL VAL ASN GLY THR ASP V1314 F1315 L1316 D1317 H1321 E1325 A1331 A1332 S1333 H1334 R1335 V1336 M1337 E1340 Y1341 N1344 LYS GLN THR HIS ALA PRO V1351 H1352 M1353 G1354 Q1355 Y1356 L1357 I1358 E1359 E1360 K1365 R1366 L1367 L1368 K1369 L1370 GLY
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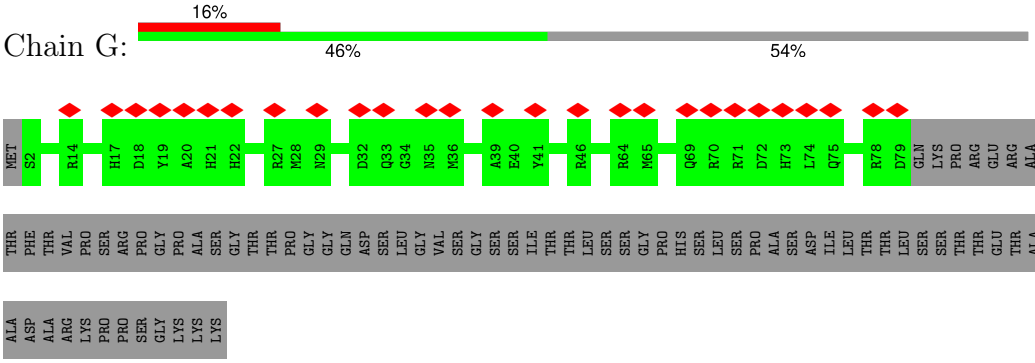
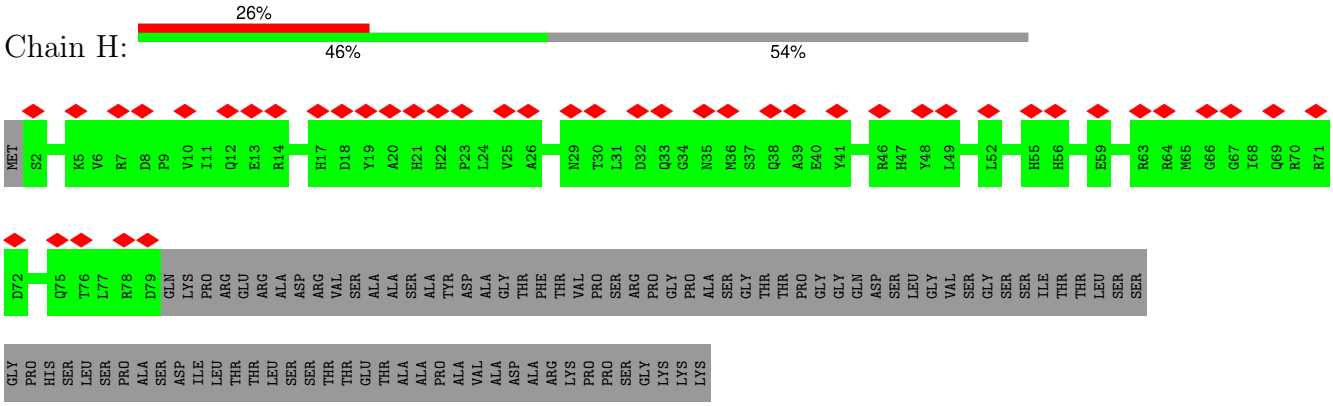
• Molecule 2: Small capsomere-interacting protein

Chain G:



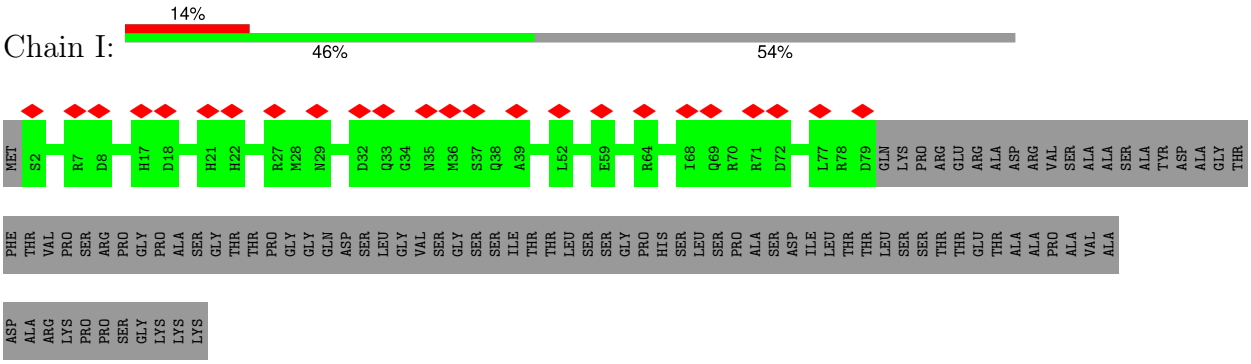
• Molecule 2: Small capsomere-interacting protein

Chain H:



• Molecule 2: Small capsomere-interacting protein

Chain I:



• Molecule 2: Small capsomere-interacting protein

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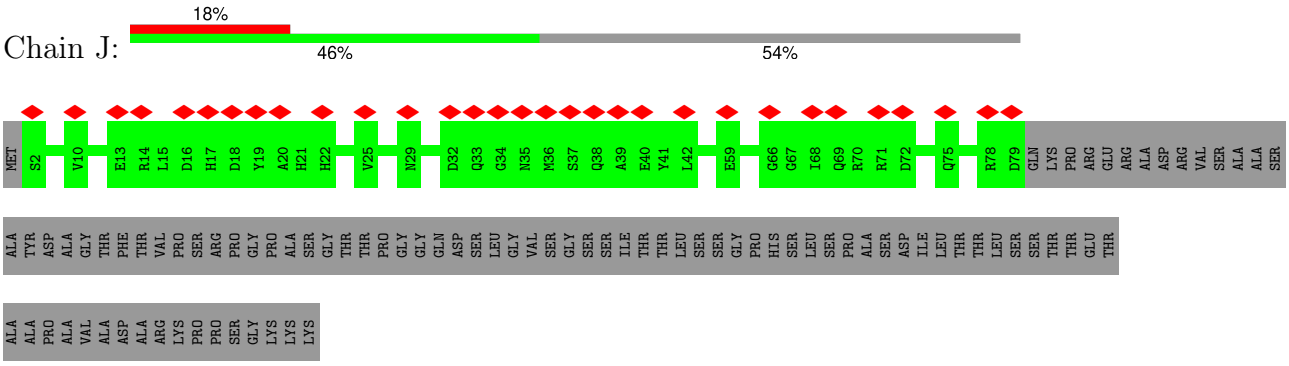
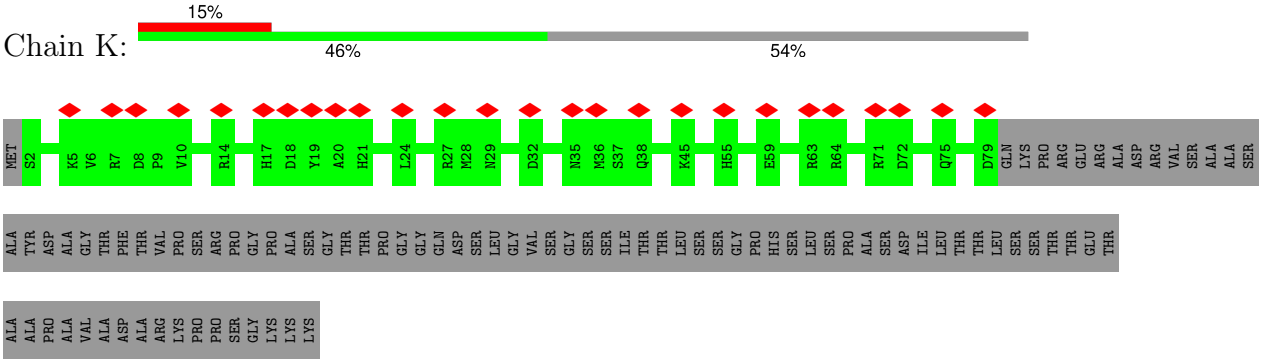


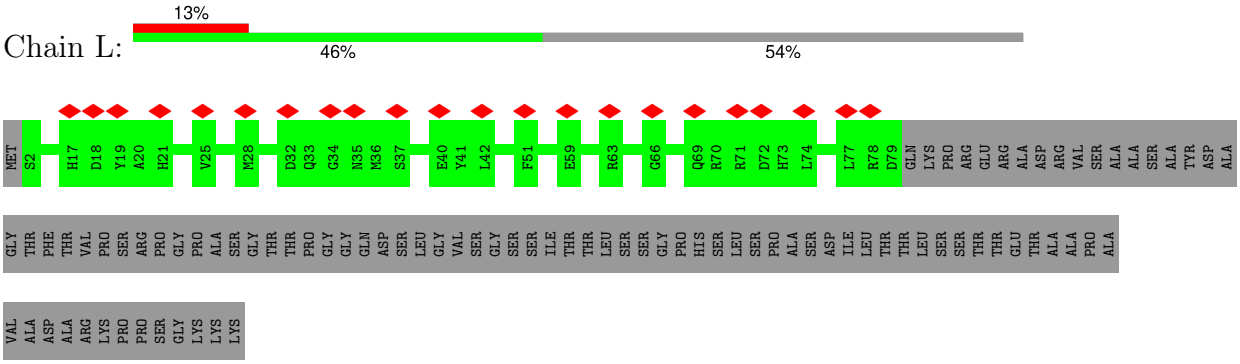
• Molecule 2: Small capsomere-interacting protein

Chain K:



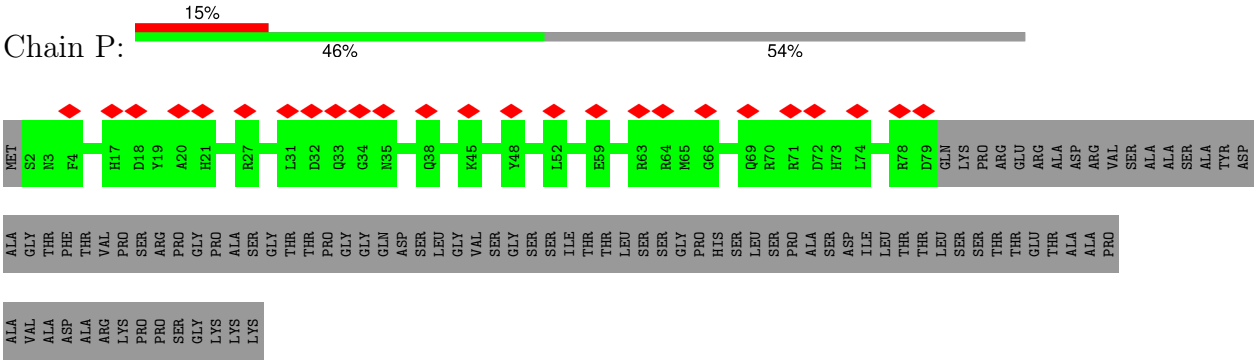
• Molecule 2: Small capsomere-interacting protein

Chain L:



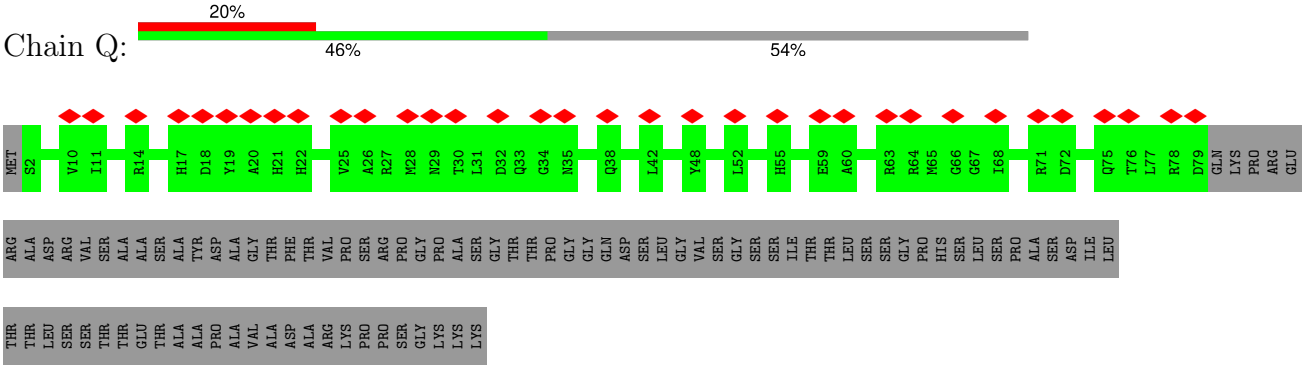
• Molecule 2: Small capsomere-interacting protein

Chain P:



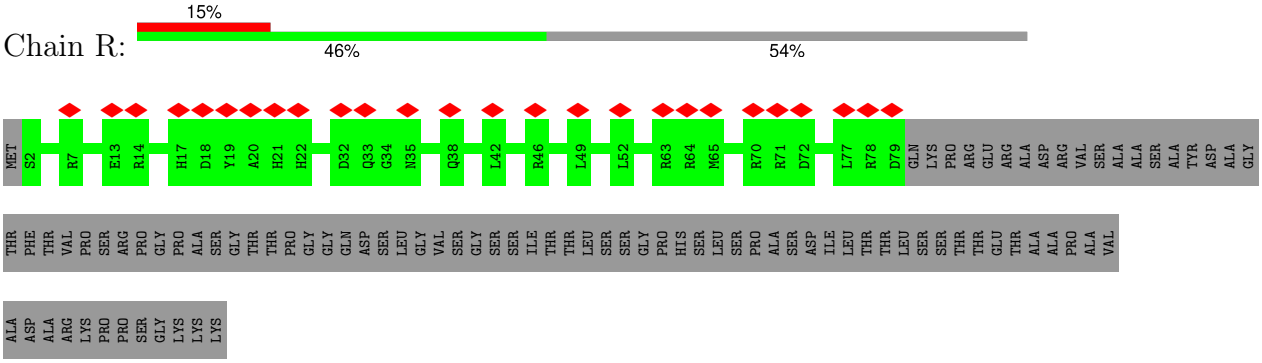
• Molecule 2: Small capsomere-interacting protein

Chain Q:



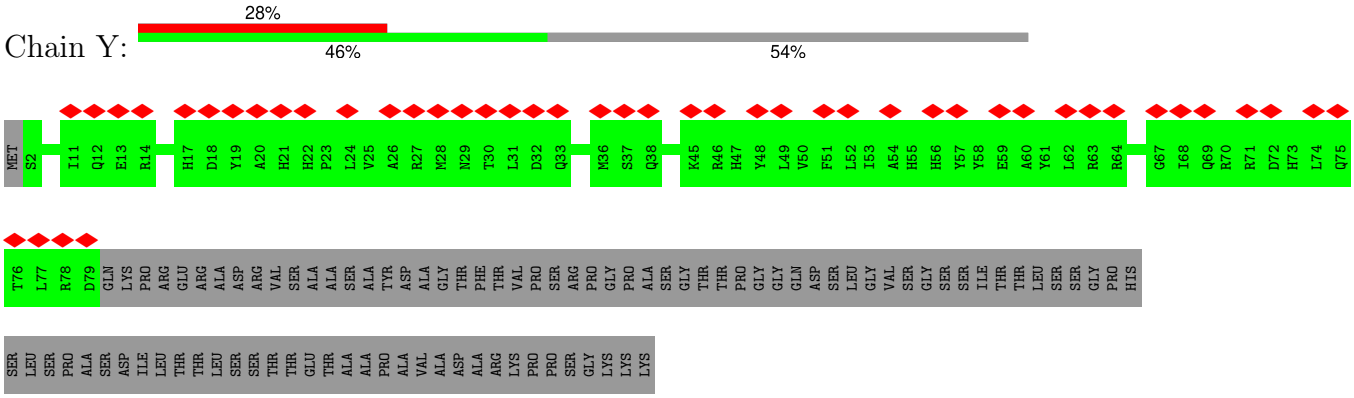
• Molecule 2: Small capsomere-interacting protein

Chain R:



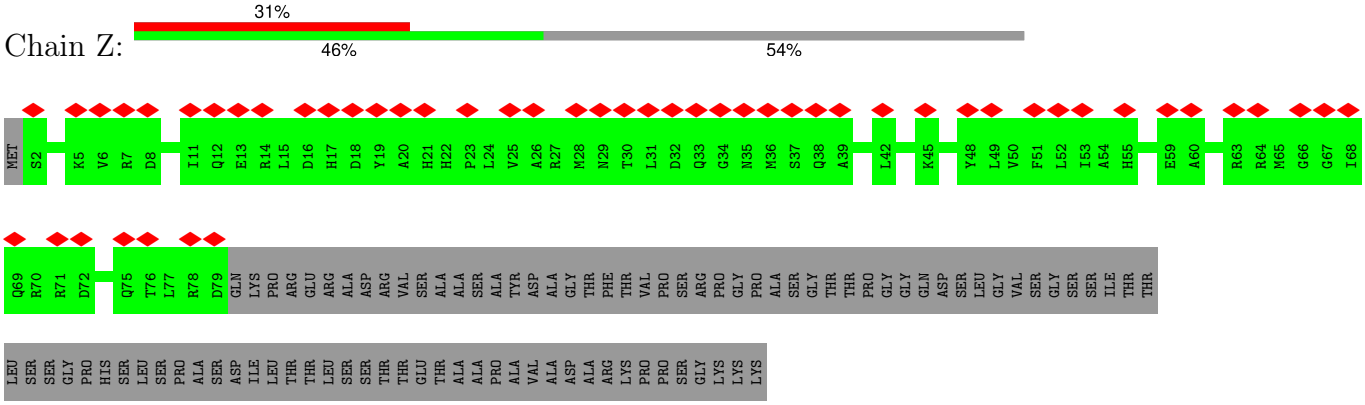
• Molecule 2: Small capsomere-interacting protein

Chain Y:



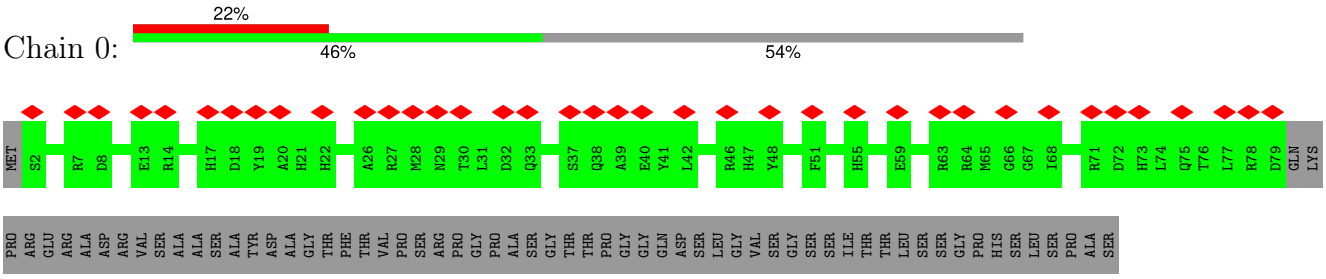
• Molecule 2: Small capsomere-interacting protein

Chain Z:



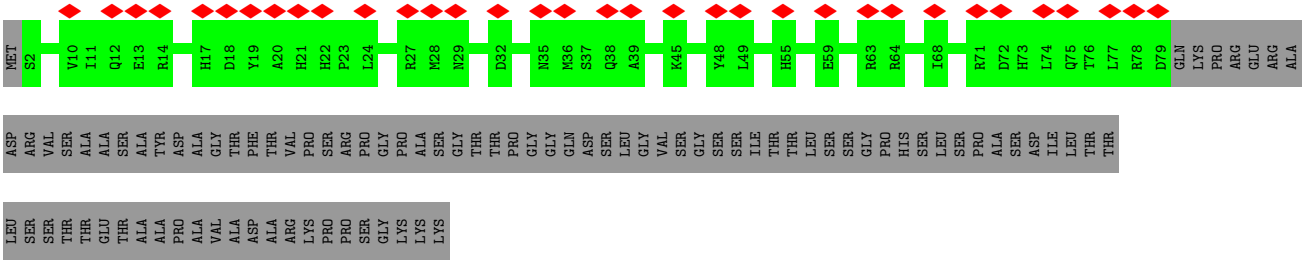
• Molecule 2: Small capsomere-interacting protein

Chain 0:



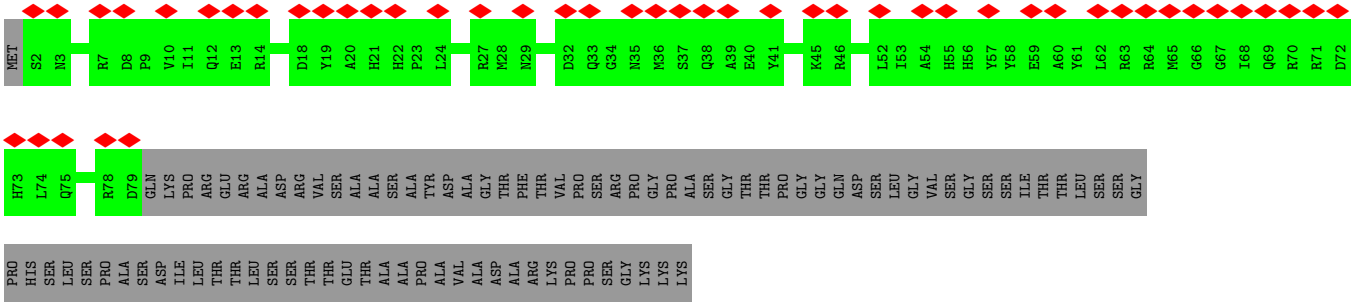
• Molecule 2: Small capsomere-interacting protein

Chain 1:



• Molecule 2: Small capsomere-interacting protein

Chain 2:



• Molecule 2: Small capsomere-interacting protein

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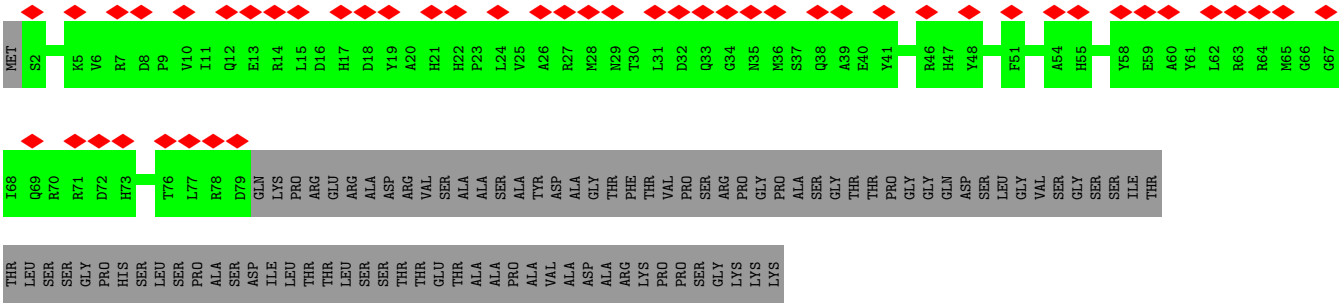
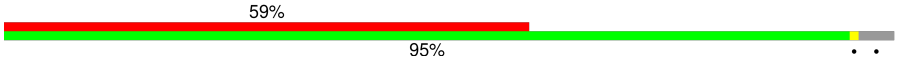
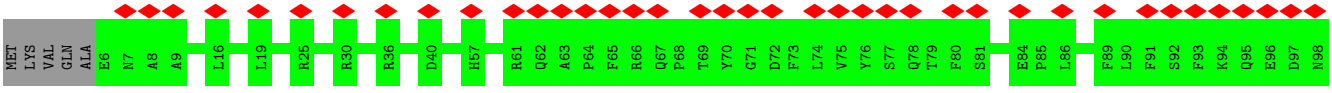
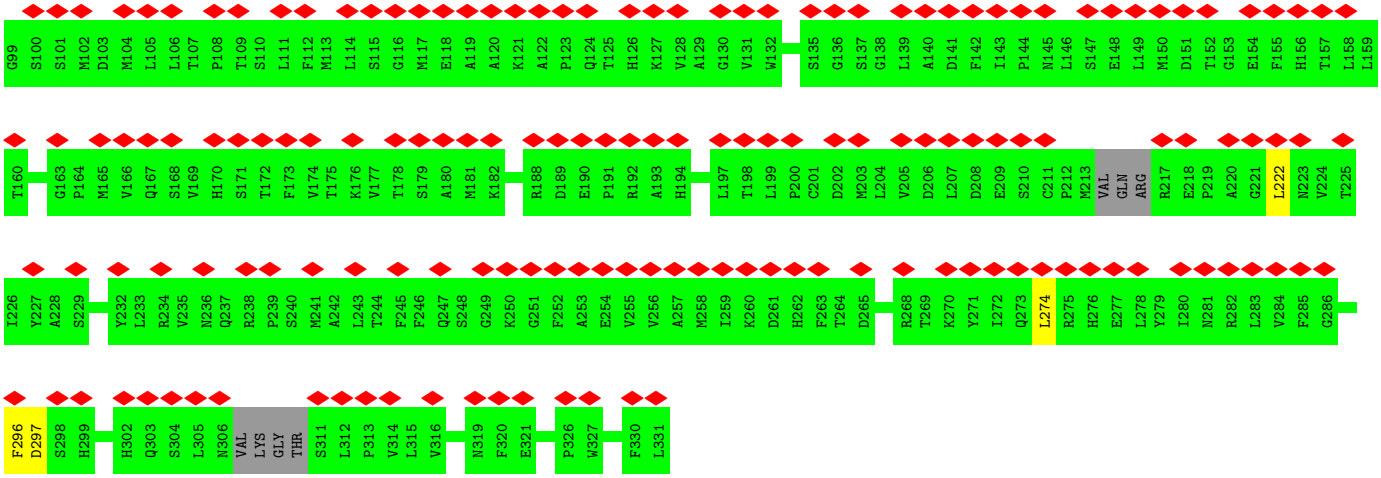


• Molecule 3: Triplex capsid protein 1

Chain 5:

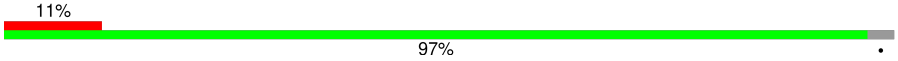


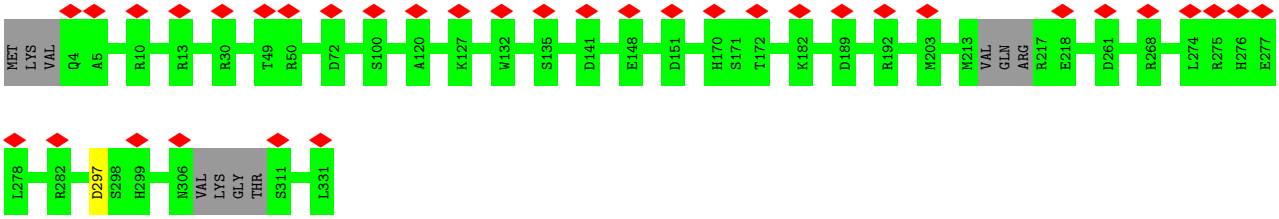




• Molecule 3: Triplex capsid protein 1

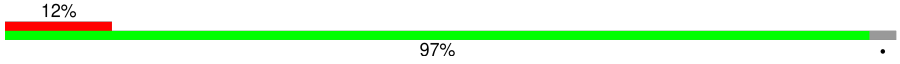
Chain 8:

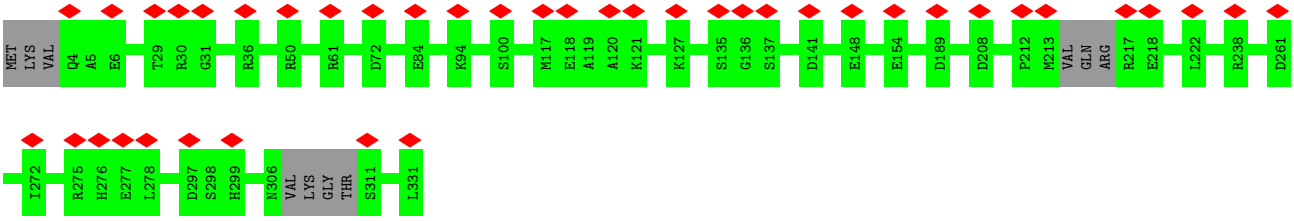




• Molecule 3: Triplex capsid protein 1

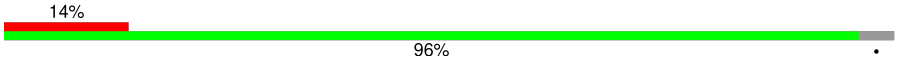
Chain b:

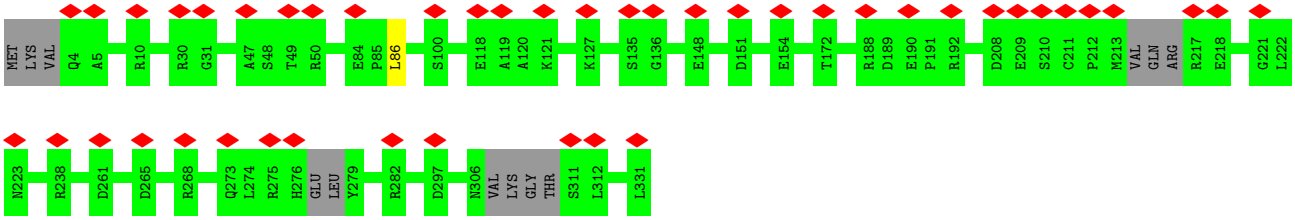




• Molecule 3: Triplex capsid protein 1

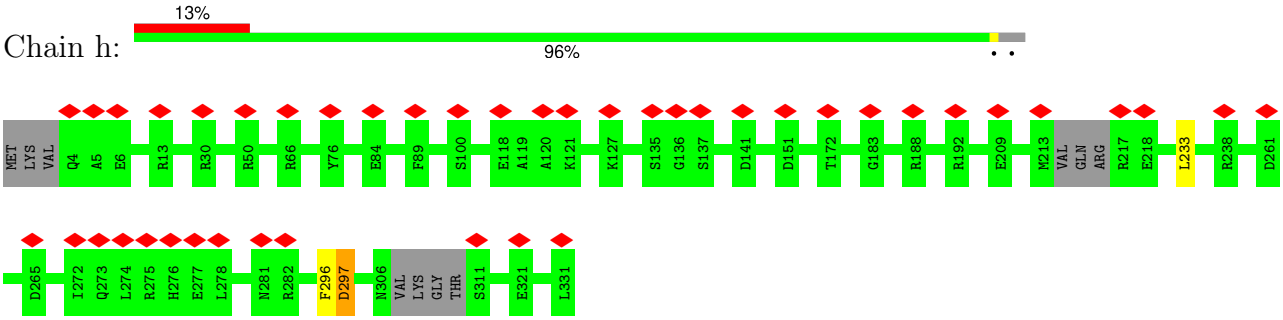
Chain e:





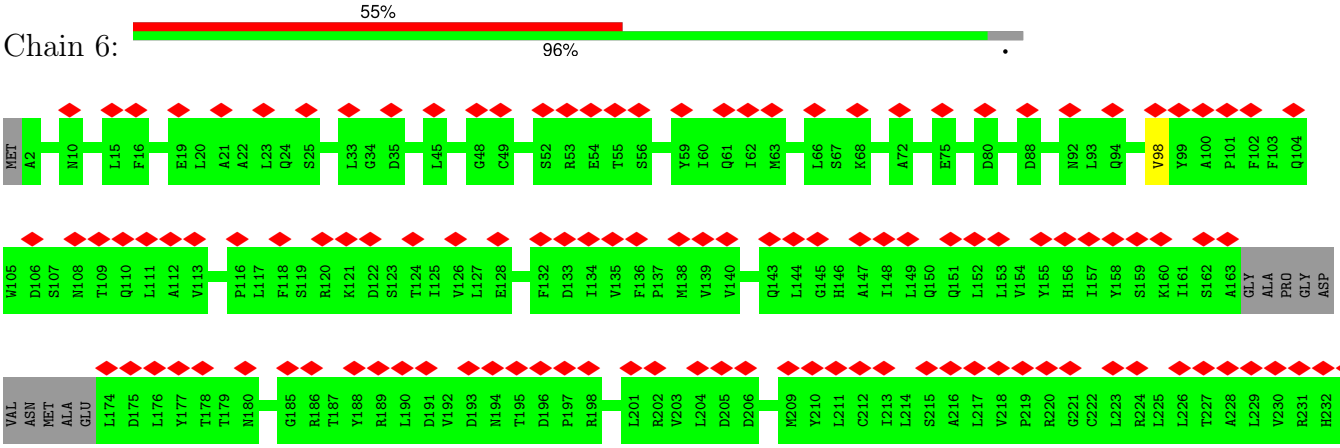
• Molecule 3: Triplex capsid protein 1

Chain h:



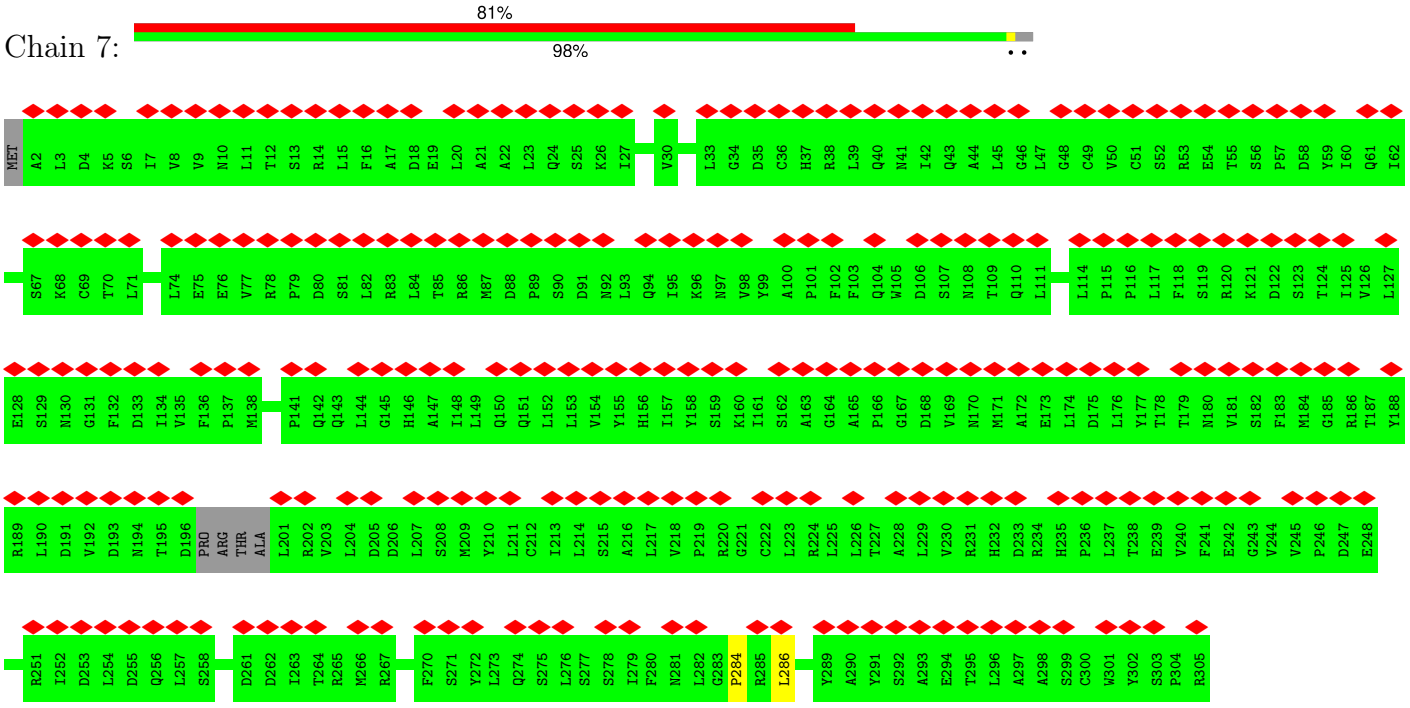
• Molecule 4: Triplex capsid protein 2

Chain 6:



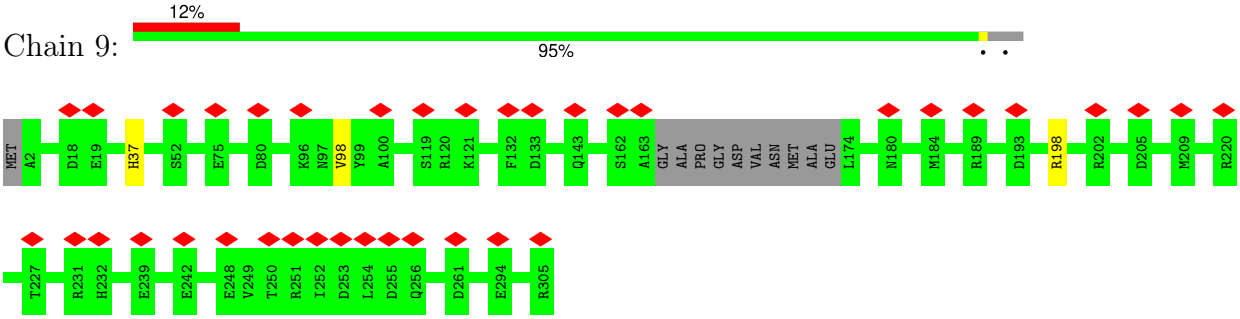
• Molecule 4: Triplex capsid protein 2

Chain 7:



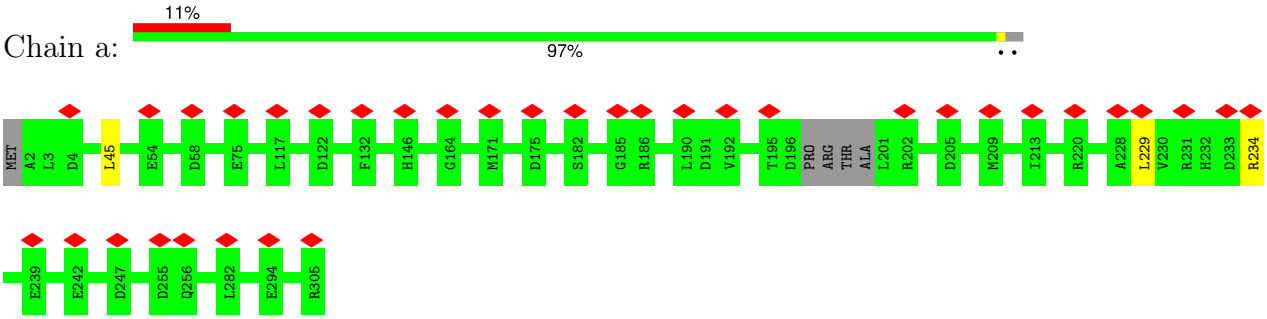
• Molecule 4: Triplex capsid protein 2

Chain 9:



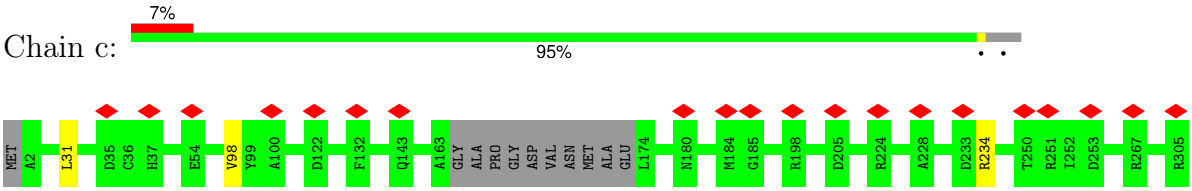
• Molecule 4: Triplex capsid protein 2

Chain a:



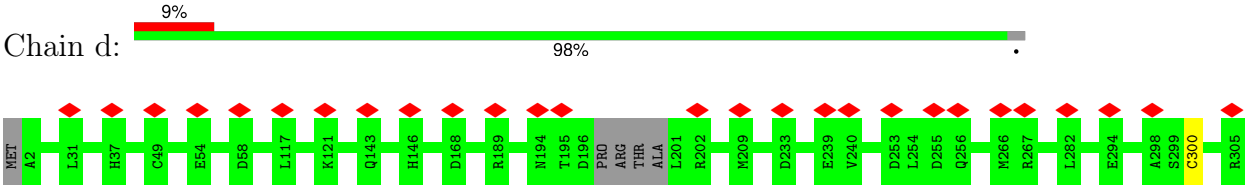
• Molecule 4: Triplex capsid protein 2

Chain c:



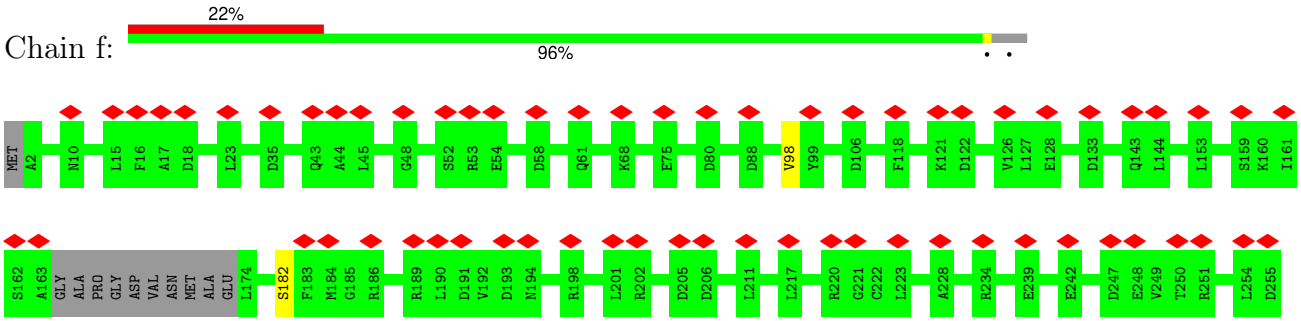
• Molecule 4: Triplex capsid protein 2

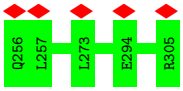
Chain d:



• Molecule 4: Triplex capsid protein 2

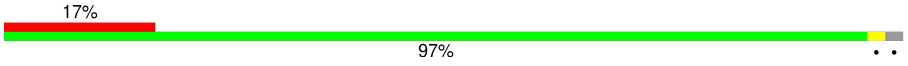
Chain f:

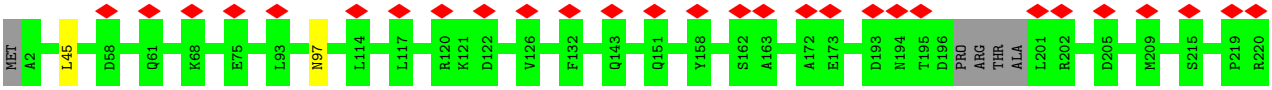


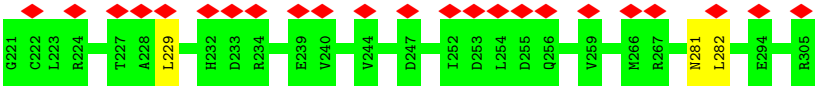


• Molecule 4: Triplex capsid protein 2

Chain g:

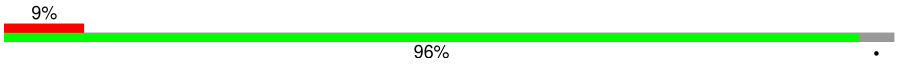


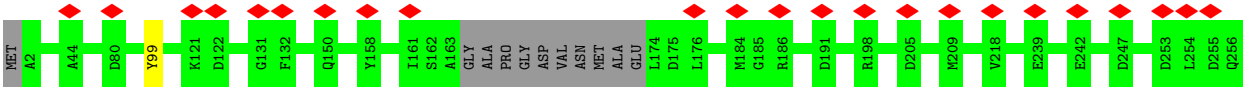


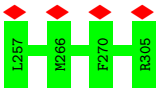


• Molecule 4: Triplex capsid protein 2

Chain i:

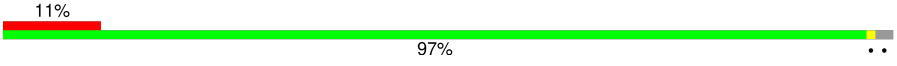


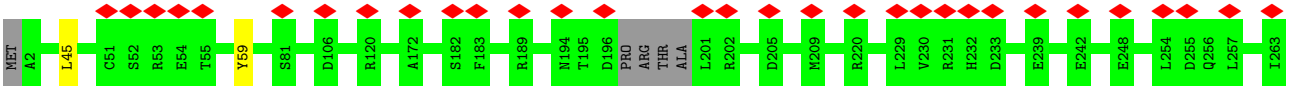


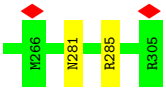


• Molecule 4: Triplex capsid protein 2

Chain j:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	25315	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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.720	Depositor
Minimum map value	-11.596	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.070	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	1318.3999, 1318.3999, 1318.3999	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	4	0.34	0/9812	0.62	3/13326 (0.0%)
1	A	0.42	0/10936	0.64	4/14866 (0.0%)
1	B	0.44	0/10879	0.67	4/14788 (0.0%)
1	C	0.43	0/10873	0.64	7/14780 (0.0%)
1	D	0.43	1/10879 (0.0%)	0.66	4/14788 (0.0%)
1	E	0.45	1/10936 (0.0%)	0.66	3/14866 (0.0%)
1	F	0.44	1/10890 (0.0%)	0.66	4/14802 (0.0%)
1	M	0.44	0/10879	0.66	3/14788 (0.0%)
1	N	0.45	1/10936 (0.0%)	0.67	5/14866 (0.0%)
1	O	0.44	0/10879	0.66	3/14788 (0.0%)
1	S	0.40	0/10298	0.64	3/13995 (0.0%)
1	T	0.42	0/10918	0.65	2/14839 (0.0%)
1	U	0.44	0/10879	0.65	1/14788 (0.0%)
1	V	0.43	0/10856	0.66	5/14757 (0.0%)
1	W	0.43	3/10873 (0.0%)	0.65	7/14780 (0.0%)
1	X	0.40	0/10797	0.64	5/14676 (0.0%)
2	0	0.37	0/682	0.52	0/919
2	1	0.38	0/682	0.52	0/919
2	2	0.37	0/682	0.52	0/919
2	3	0.37	0/682	0.52	0/919
2	G	0.38	0/682	0.52	0/919
2	H	0.37	0/682	0.52	0/919
2	I	0.37	0/682	0.52	0/919
2	J	0.37	0/682	0.52	0/919
2	K	0.38	0/682	0.52	0/919
2	L	0.37	0/682	0.52	0/919
2	P	0.37	0/682	0.52	0/919
2	Q	0.37	0/682	0.52	0/919
2	R	0.38	0/682	0.52	0/919
2	Y	0.37	0/682	0.52	0/919
2	Z	0.37	0/682	0.52	0/919
3	5	0.33	0/2525	0.62	4/3433 (0.1%)
3	8	0.41	0/2539	0.63	1/3452 (0.0%)
3	b	0.41	0/2539	0.63	0/3452

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	e	0.40	0/2521	0.62	1/3426 (0.0%)
3	h	0.41	0/2539	0.64	2/3452 (0.1%)
4	6	0.34	0/2375	0.65	0/3234
4	7	0.33	0/2410	0.61	1/3281 (0.0%)
4	9	0.43	0/2375	0.66	0/3234
4	a	0.45	1/2410 (0.0%)	0.65	1/3281 (0.0%)
4	c	0.43	0/2375	0.67	1/3234 (0.0%)
4	d	0.44	0/2410	0.64	0/3281
4	f	0.38	0/2375	0.65	0/3234
4	g	0.41	0/2410	0.66	2/3281 (0.1%)
4	i	0.42	0/2375	0.65	0/3234
4	j	0.43	0/2410	0.66	2/3281 (0.1%)
All	All	0.42	8/219338 (0.0%)	0.65	78/298068 (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
1	4	0	9
1	A	0	4
1	B	0	7
1	C	0	8
1	D	0	10
1	E	0	5
1	F	0	4
1	M	0	6
1	N	0	7
1	O	0	6
1	S	0	6
1	T	0	11
1	U	0	4
1	V	0	6
1	W	0	2
1	X	0	1
3	h	0	1
4	6	0	1
4	7	0	1
4	9	0	2
4	a	0	1
4	c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	1
4	f	0	2
4	g	0	2
4	i	0	1
4	j	0	2
All	All	0	111

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	454	CYS	C-N	-7.03	1.17	1.34
4	a	234	ARG	CZ-NH2	-6.59	1.24	1.33
1	W	964	TYR	CD1-CE1	-6.35	1.29	1.39
1	N	9	PRO	C-N	-6.01	1.20	1.34
1	E	1192	GLN	C-N	-5.61	1.21	1.34

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1181	PRO	C-N-CA	10.87	148.86	121.70
1	B	1232	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	X	5	LEU	CA-CB-CG	8.38	134.58	115.30
1	B	1232	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	F	454	CYS	C-N-CA	8.04	141.80	121.70

There are no chirality outliers.

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1109	THR	Peptide
1	A	255	ASP	Peptide
1	A	537	HIS	Peptide
1	A	899	ASP	Peptide
1	B	422	VAL	Peptide

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	4	1200/1376 (87%)	1061 (88%)	136 (11%)	3 (0%)	37	71
1	A	1359/1376 (99%)	1204 (89%)	155 (11%)	0	100	100
1	B	1351/1376 (98%)	1192 (88%)	158 (12%)	1 (0%)	48	82
1	C	1350/1376 (98%)	1200 (89%)	148 (11%)	2 (0%)	48	82
1	D	1351/1376 (98%)	1186 (88%)	163 (12%)	2 (0%)	48	82
1	E	1359/1376 (99%)	1203 (88%)	155 (11%)	1 (0%)	48	82
1	F	1352/1376 (98%)	1197 (88%)	149 (11%)	6 (0%)	30	67
1	M	1351/1376 (98%)	1185 (88%)	163 (12%)	3 (0%)	44	77
1	N	1359/1376 (99%)	1189 (88%)	168 (12%)	2 (0%)	48	82
1	O	1351/1376 (98%)	1191 (88%)	155 (12%)	5 (0%)	30	67
1	S	1273/1376 (92%)	1126 (88%)	145 (11%)	2 (0%)	44	77
1	T	1354/1376 (98%)	1195 (88%)	154 (11%)	5 (0%)	30	67
1	U	1351/1376 (98%)	1199 (89%)	150 (11%)	2 (0%)	48	82
1	V	1348/1376 (98%)	1200 (89%)	146 (11%)	2 (0%)	48	82
1	W	1350/1376 (98%)	1211 (90%)	136 (10%)	3 (0%)	44	77
1	X	1339/1376 (97%)	1198 (90%)	140 (10%)	1 (0%)	48	82
2	0	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	1	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	2	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	3	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	G	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	H	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	I	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	J	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	K	76/170 (45%)	73 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	P	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Q	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	R	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Y	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Z	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
3	5	313/331 (95%)	279 (89%)	34 (11%)	0	100	100
3	8	315/331 (95%)	293 (93%)	22 (7%)	0	100	100
3	b	315/331 (95%)	288 (91%)	27 (9%)	0	100	100
3	e	311/331 (94%)	288 (93%)	23 (7%)	0	100	100
3	h	315/331 (95%)	288 (91%)	26 (8%)	1 (0%)	37	71
4	6	290/305 (95%)	263 (91%)	27 (9%)	0	100	100
4	7	296/305 (97%)	261 (88%)	35 (12%)	0	100	100
4	9	290/305 (95%)	264 (91%)	26 (9%)	0	100	100
4	a	296/305 (97%)	270 (91%)	26 (9%)	0	100	100
4	c	290/305 (95%)	265 (91%)	25 (9%)	0	100	100
4	d	296/305 (97%)	277 (94%)	19 (6%)	0	100	100
4	f	290/305 (95%)	263 (91%)	27 (9%)	0	100	100
4	g	296/305 (97%)	269 (91%)	27 (9%)	0	100	100
4	i	290/305 (95%)	264 (91%)	26 (9%)	0	100	100
4	j	296/305 (97%)	272 (92%)	24 (8%)	0	100	100
All	All	27037/29271 (92%)	24136 (89%)	2860 (11%)	41 (0%)	45	77

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1251	ASN
1	O	144	GLU
1	T	10	PHE
1	V	1251	ASN
1	B	843	VAL

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	4	1039/1166 (89%)	1038 (100%)	1 (0%)	92 94
1	A	1155/1166 (99%)	1155 (100%)	0	100 100
1	B	1151/1166 (99%)	1150 (100%)	1 (0%)	92 94
1	C	1150/1166 (99%)	1150 (100%)	0	100 100
1	D	1151/1166 (99%)	1151 (100%)	0	100 100
1	E	1155/1166 (99%)	1155 (100%)	0	100 100
1	F	1152/1166 (99%)	1151 (100%)	1 (0%)	92 94
1	M	1151/1166 (99%)	1151 (100%)	0	100 100
1	N	1155/1166 (99%)	1153 (100%)	2 (0%)	92 94
1	O	1151/1166 (99%)	1149 (100%)	2 (0%)	92 94
1	S	1094/1166 (94%)	1094 (100%)	0	100 100
1	T	1154/1166 (99%)	1153 (100%)	1 (0%)	92 94
1	U	1151/1166 (99%)	1149 (100%)	2 (0%)	92 94
1	V	1148/1166 (98%)	1146 (100%)	2 (0%)	92 94
1	W	1150/1166 (99%)	1150 (100%)	0	100 100
1	X	1143/1166 (98%)	1143 (100%)	0	100 100
2	0	70/141 (50%)	70 (100%)	0	100 100
2	1	70/141 (50%)	70 (100%)	0	100 100
2	2	70/141 (50%)	70 (100%)	0	100 100
2	3	70/141 (50%)	70 (100%)	0	100 100
2	G	70/141 (50%)	70 (100%)	0	100 100
2	H	70/141 (50%)	70 (100%)	0	100 100
2	I	70/141 (50%)	70 (100%)	0	100 100
2	J	70/141 (50%)	70 (100%)	0	100 100
2	K	70/141 (50%)	70 (100%)	0	100 100
2	L	70/141 (50%)	70 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	70/141 (50%)	70 (100%)	0	100	100
2	Q	70/141 (50%)	70 (100%)	0	100	100
2	R	70/141 (50%)	70 (100%)	0	100	100
2	Y	70/141 (50%)	70 (100%)	0	100	100
2	Z	70/141 (50%)	70 (100%)	0	100	100
3	5	271/281 (96%)	271 (100%)	0	100	100
3	8	272/281 (97%)	272 (100%)	0	100	100
3	b	272/281 (97%)	272 (100%)	0	100	100
3	e	270/281 (96%)	270 (100%)	0	100	100
3	h	272/281 (97%)	272 (100%)	0	100	100
4	6	267/274 (97%)	267 (100%)	0	100	100
4	7	270/274 (98%)	270 (100%)	0	100	100
4	9	267/274 (97%)	266 (100%)	1 (0%)	89	91
4	a	270/274 (98%)	270 (100%)	0	100	100
4	c	267/274 (97%)	266 (100%)	1 (0%)	89	91
4	d	270/274 (98%)	270 (100%)	0	100	100
4	f	267/274 (97%)	267 (100%)	0	100	100
4	g	270/274 (98%)	269 (100%)	1 (0%)	89	91
4	i	267/274 (97%)	267 (100%)	0	100	100
4	j	270/274 (98%)	270 (100%)	0	100	100
All	All	23342/24916 (94%)	23327 (100%)	15 (0%)	92	94

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	84	ARG
4	c	234	ARG
1	U	143	LYS
4	g	281	ASN
1	4	947	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 354 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	102	HIS
2	2	73	HIS
1	W	498	HIS
1	X	354	HIS
1	4	920	ASN

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 oligosaccharides 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	N	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	9:PRO	C	10:PHE	N	1.20
1	F	454:CYS	C	455:HIS	N	1.17

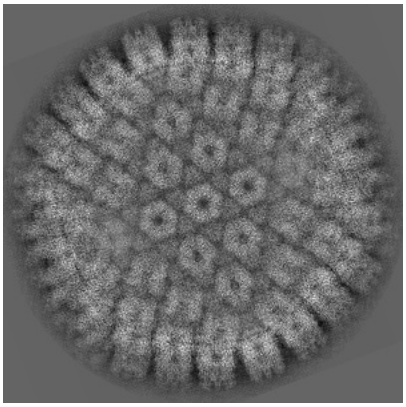
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7047. These allow visual inspection of the internal detail of the map and identification of artifacts.

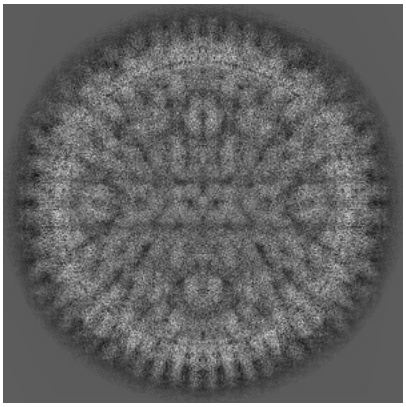
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

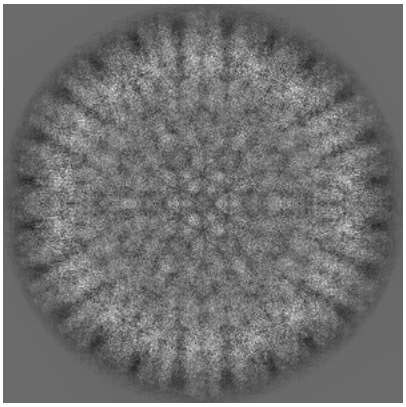
6.1.1 Primary map



X



Y

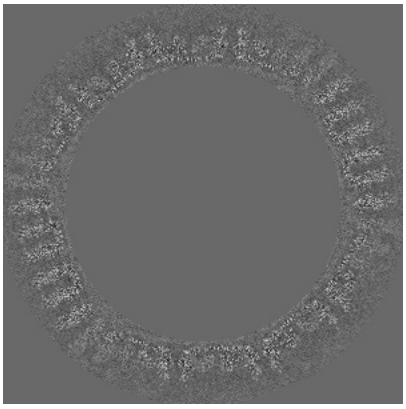


Z

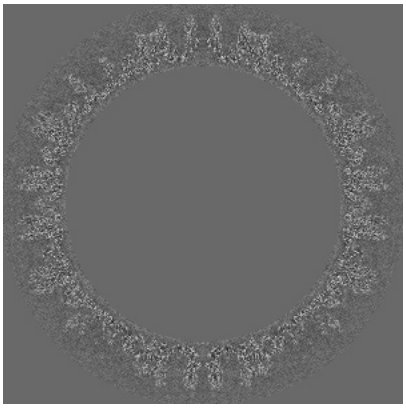
The images above show the map projected in three orthogonal directions.

6.2 Central slices

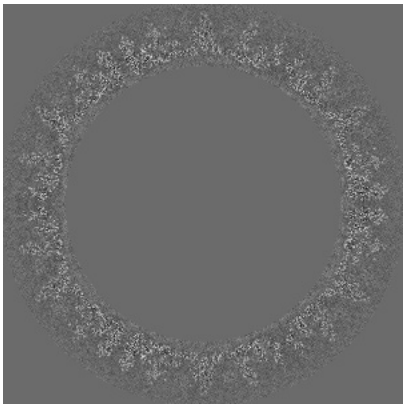
6.2.1 Primary map



X Index: 640



Y Index: 640

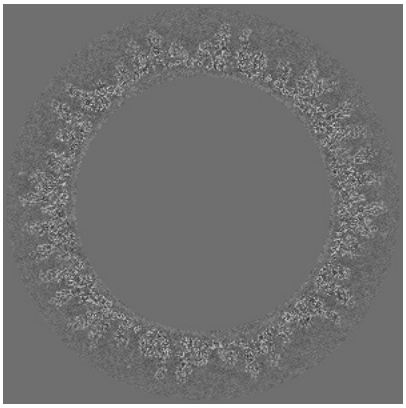


Z Index: 640

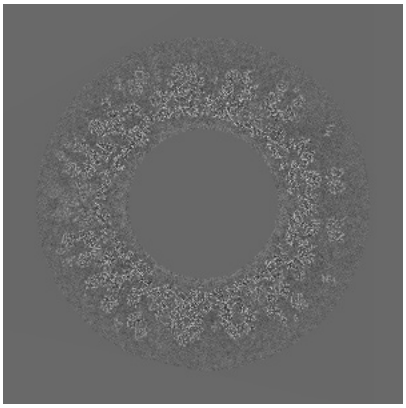
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

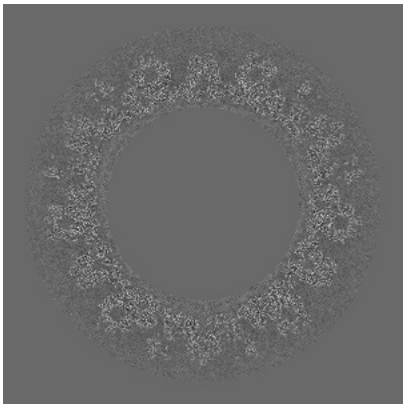
6.3.1 Primary map



X Index: 475



Y Index: 270

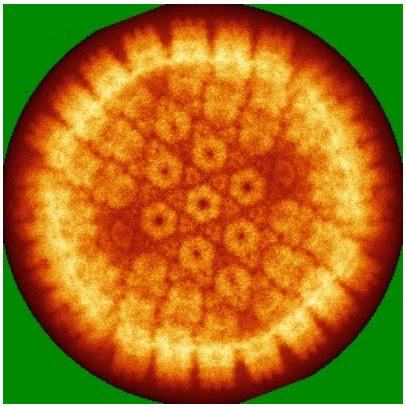


Z Index: 326

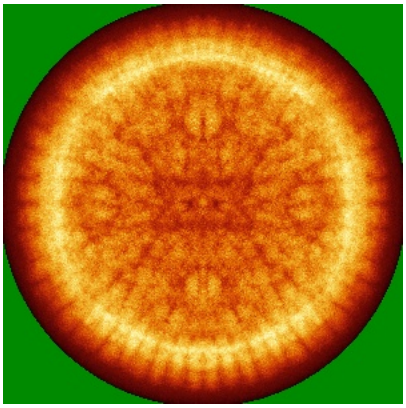
The images above show the largest variance slices of the map in three orthogonal directions.

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

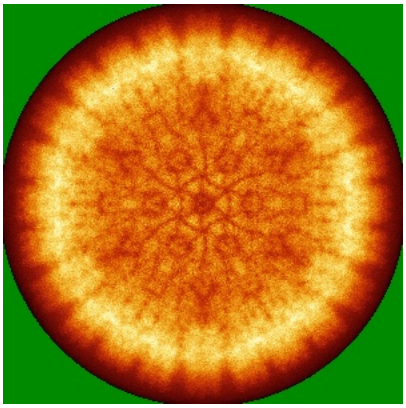
6.4.1 Primary map



X



Y



Z

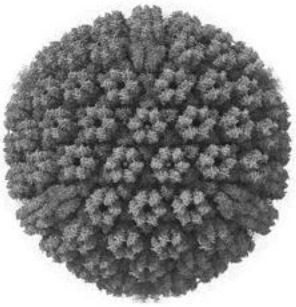
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

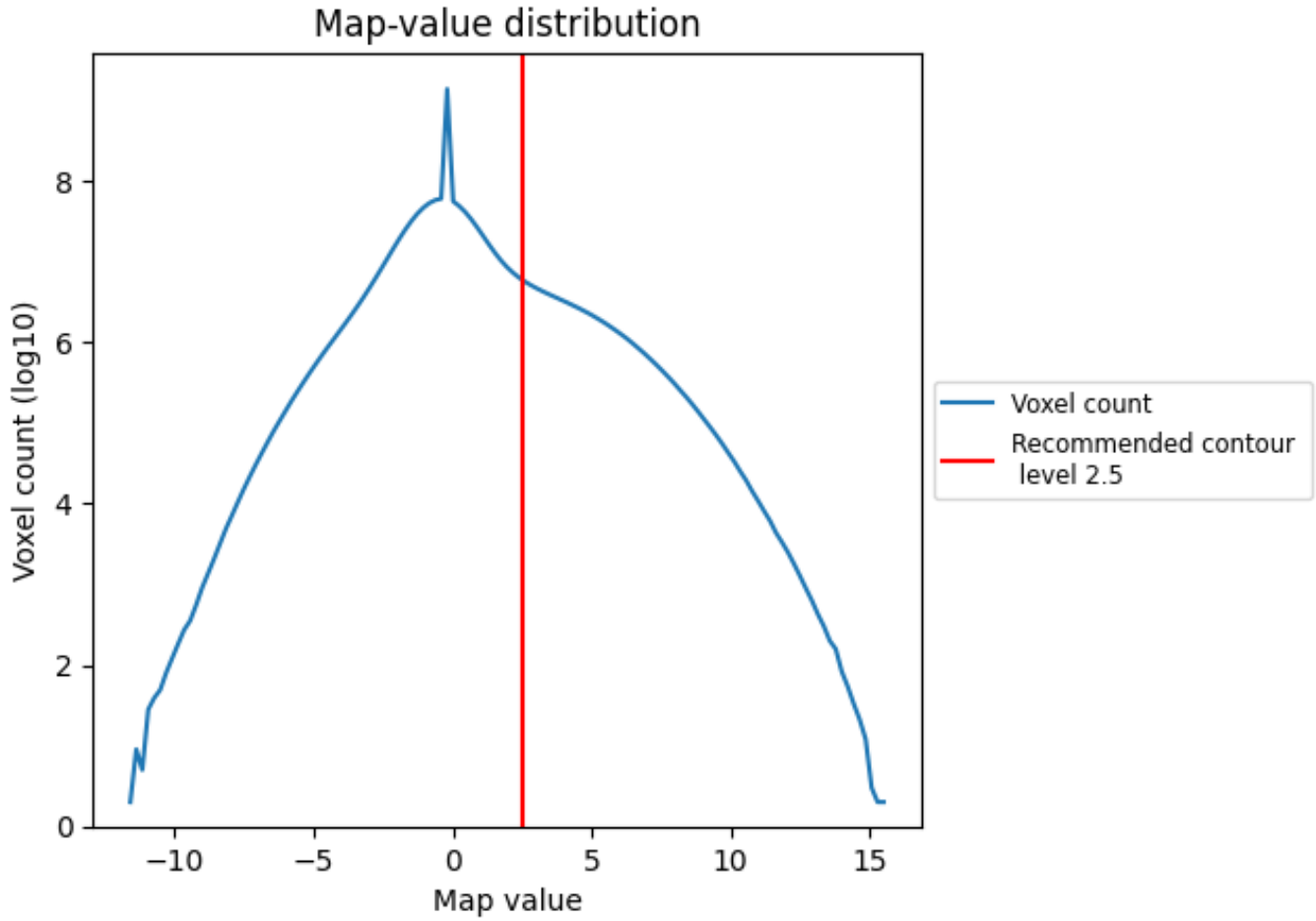
6.6 Mask visualisation (i)

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

7 Map analysis

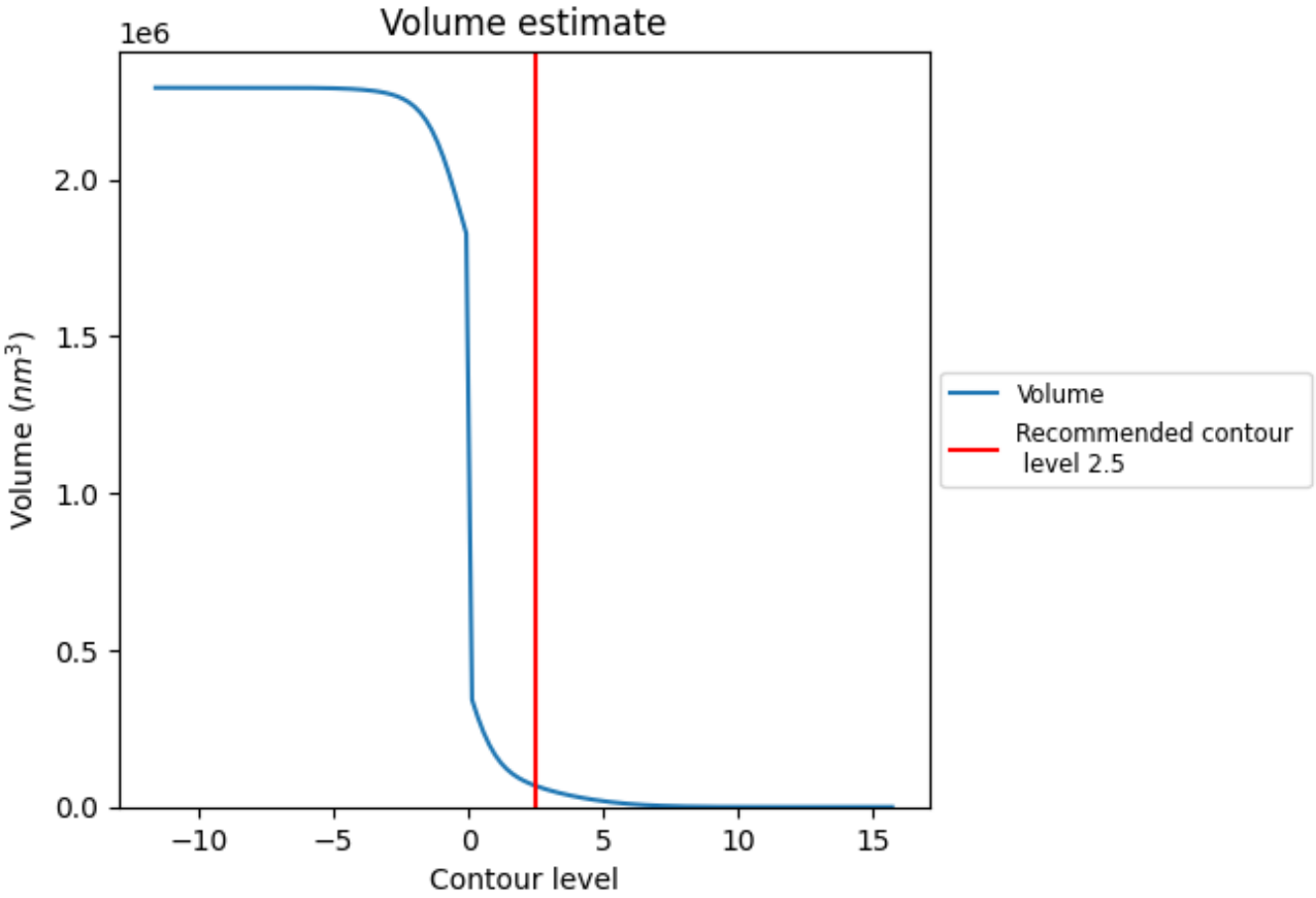
This section contains the results of statistical analysis of the map.

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.

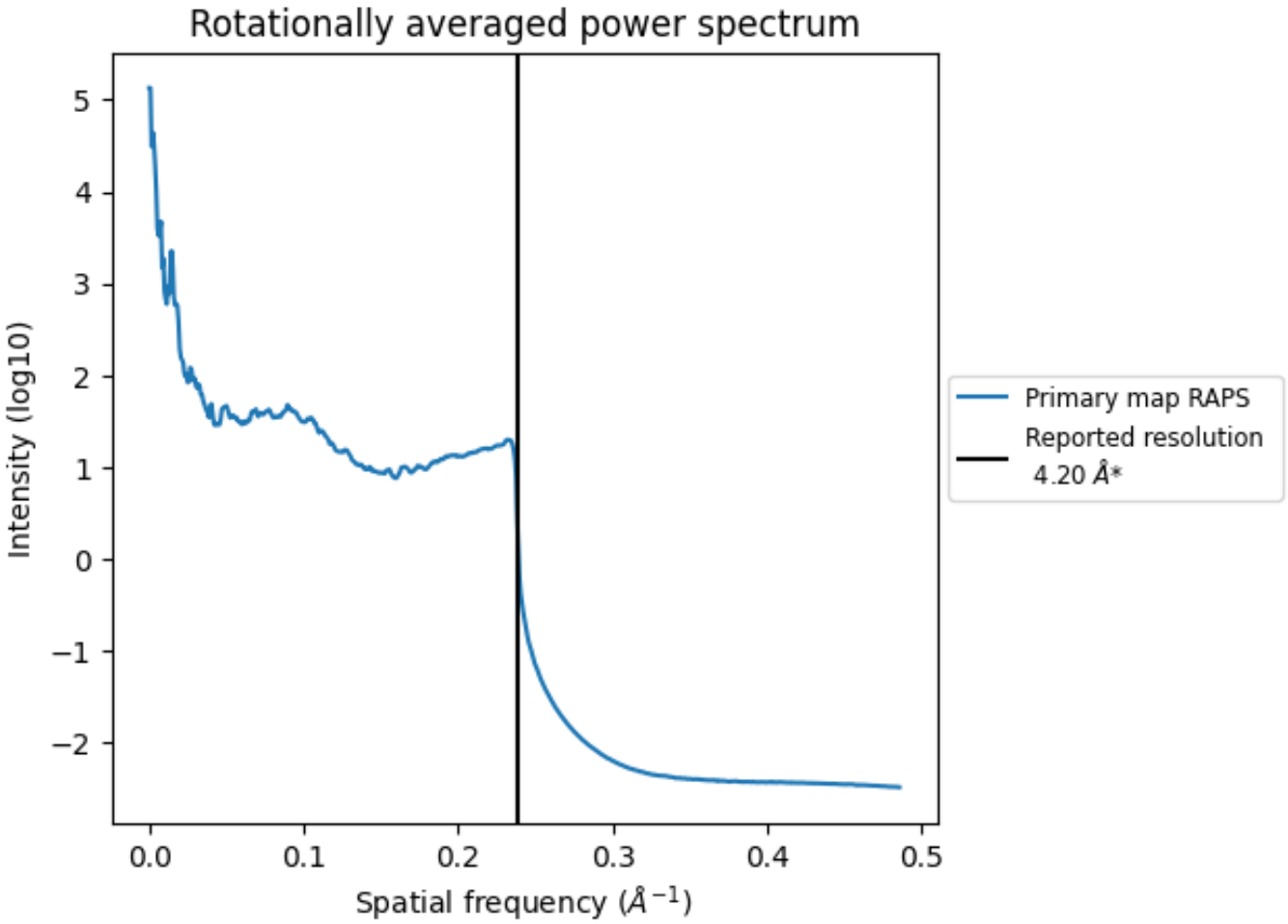
7.2 Volume estimate (i)



The volume at the recommended contour level is 67318 nm^3; this corresponds to an approximate mass of 60810 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 0.238 Å^{-1}

8 Fourier-Shell correlation

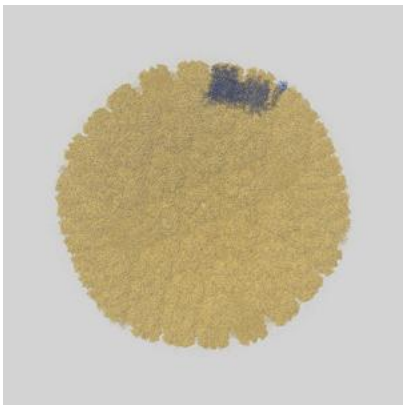
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

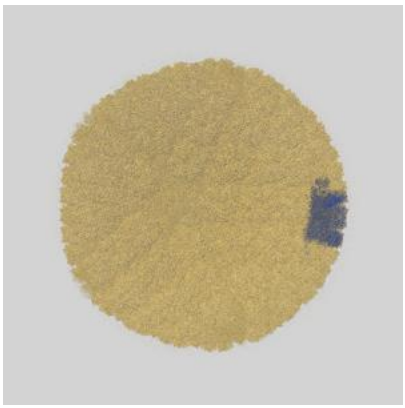
This section contains information regarding the fit between EMDB map EMD-7047 and PDB model 6B43. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

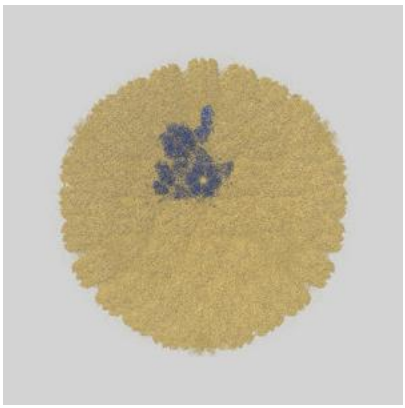
9.1.1 Map-model overlay



X

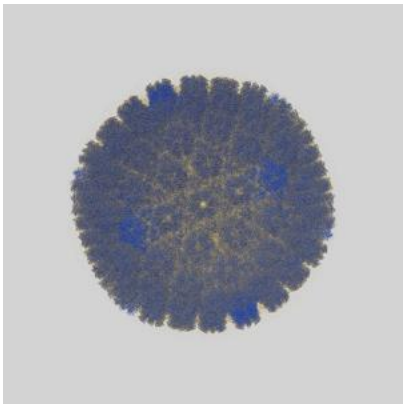


Y

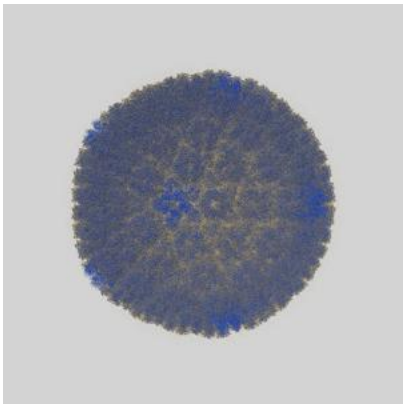


Z

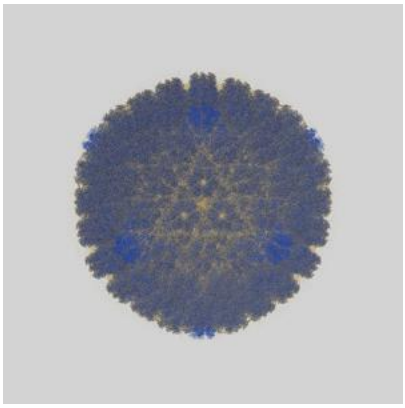
9.1.2 Map-model assembly overlay



X



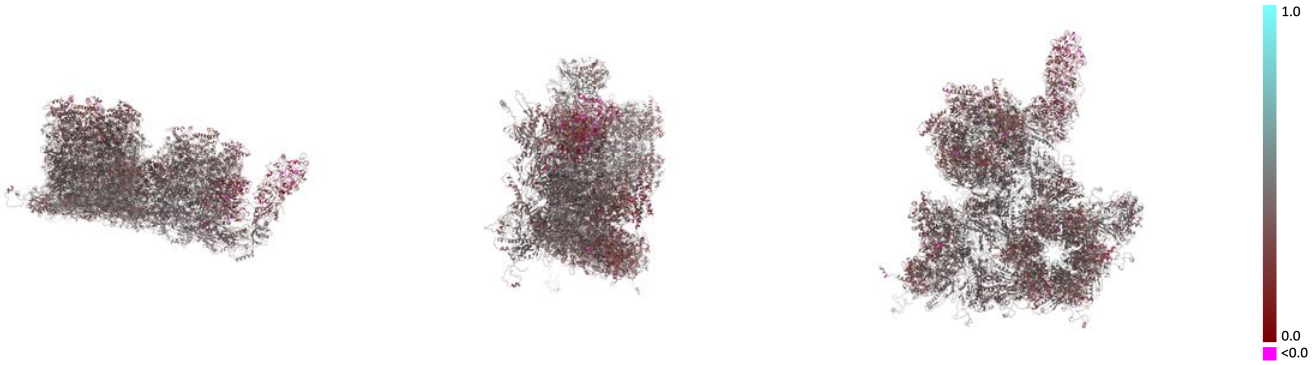
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

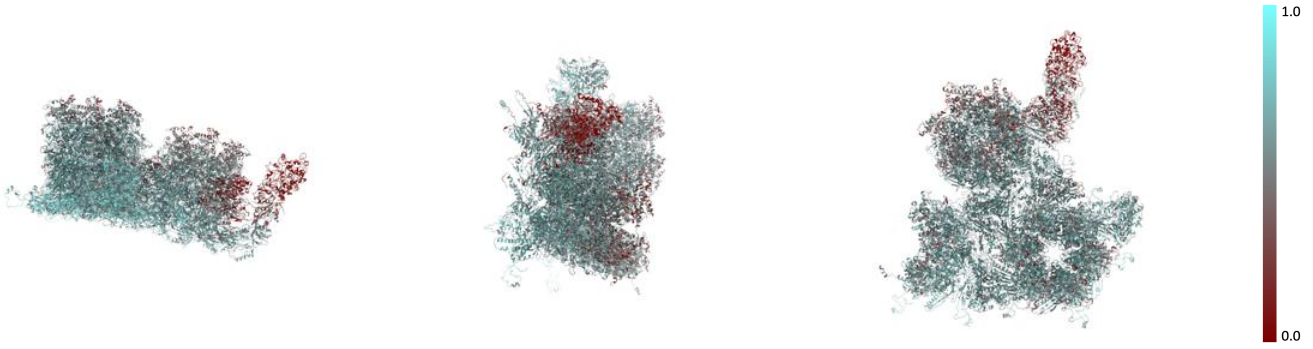
9.2 Q-score mapped to coordinate model



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.

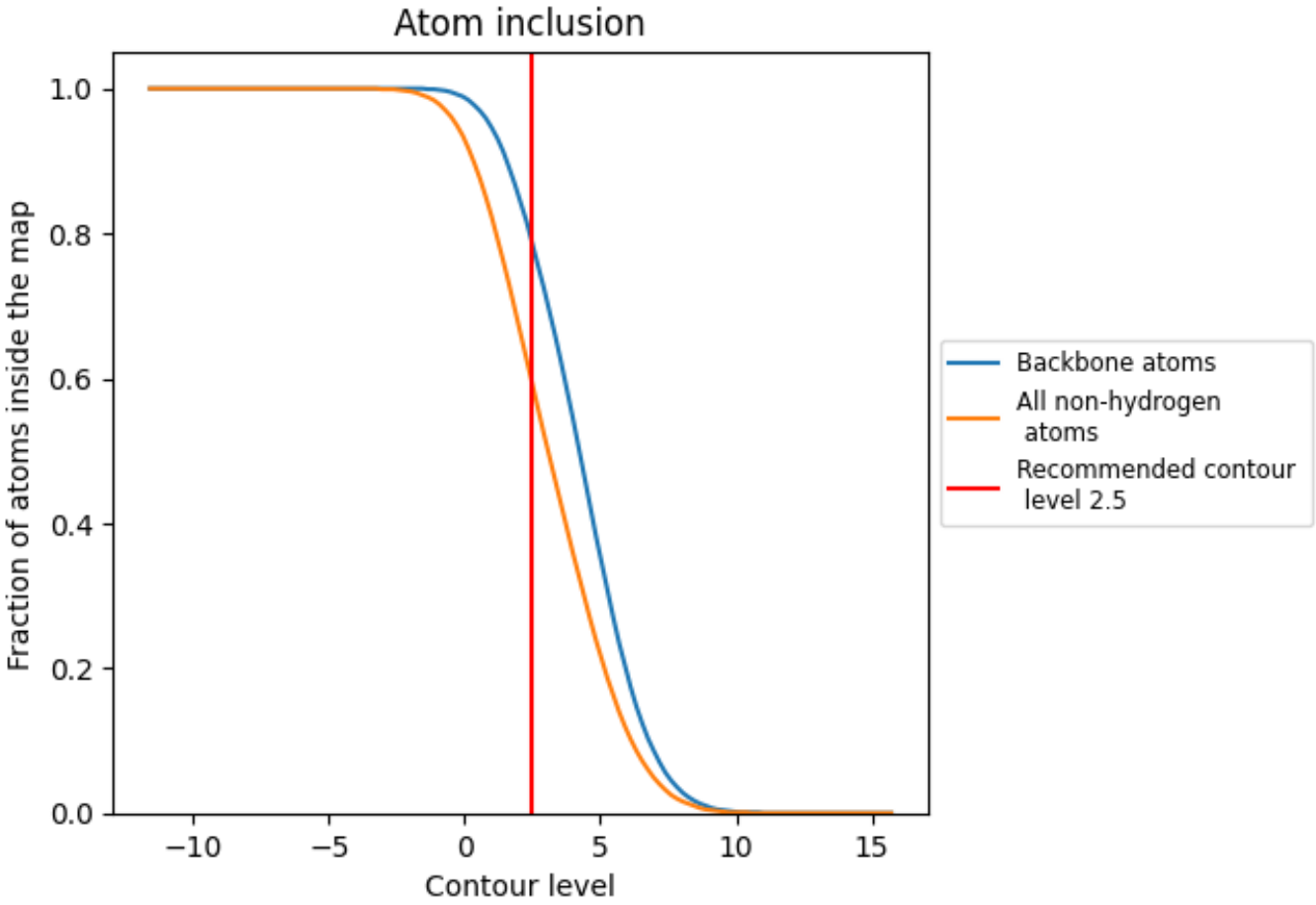
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 59% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5910	0.3760
0	0.4380	0.2910
1	0.4520	0.3070
2	0.3660	0.2610
3	0.3600	0.2470
4	0.2800	0.2860
5	0.3310	0.3130
6	0.3450	0.2850
7	0.1930	0.2500
8	0.6510	0.3990
9	0.6270	0.3870
A	0.6420	0.3980
B	0.6390	0.3880
C	0.6270	0.3870
D	0.6330	0.3840
E	0.6450	0.3990
F	0.6420	0.3960
G	0.4830	0.3050
H	0.4020	0.2270
I	0.5030	0.3280
J	0.4730	0.2980
K	0.4830	0.2990
L	0.4840	0.3170
M	0.6510	0.3990
N	0.6490	0.3980
O	0.6500	0.3960
P	0.5000	0.3220
Q	0.4840	0.2840
R	0.4950	0.2980
S	0.5690	0.3780
T	0.6080	0.3870
U	0.6240	0.3890
V	0.6210	0.3830
W	0.5950	0.3780
X	0.5730	0.3720

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Chain	Atom inclusion	Q-score
Y	0.3890	0.2760
Z	0.3520	0.2410
a	0.6350	0.3950
b	0.6460	0.4070
c	0.6560	0.3980
d	0.6500	0.3980
e	0.6140	0.3910
f	0.5620	0.3680
g	0.5930	0.3790
h	0.6380	0.3950
i	0.6420	0.3950
j	0.6410	0.3940