



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:24 AM UTC

PDB ID : 6LGL / pdb_00006lgl
EMDB ID : EMD-0880
Title : The atomic structure of varicella-zoster virus A-capsid
Authors : Zheng, Q.; Li, S.
Deposited on : 2019-12-05
Resolution : 4.40 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:

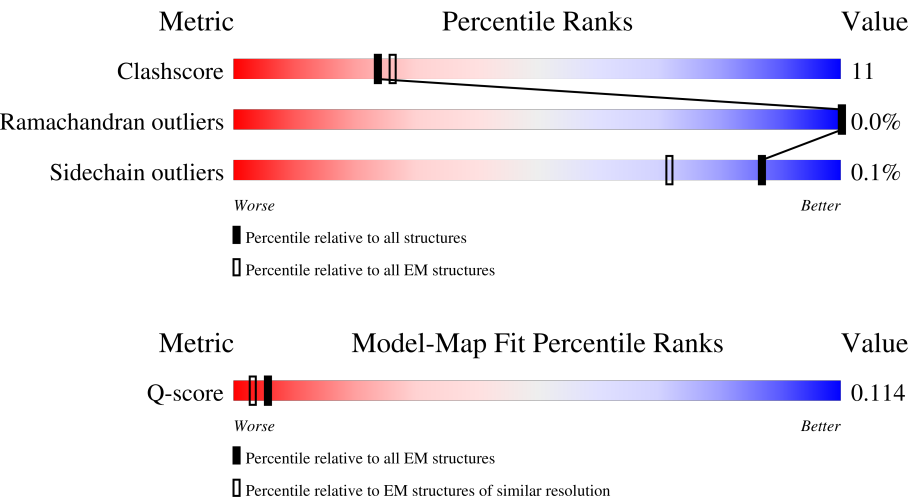
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.40 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	3132 (3.91 - 4.90)

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	1396	80%17%
1	B	1396	70%27%
1	C	1396	5%73%24%
1	E	1396	5%68%29%

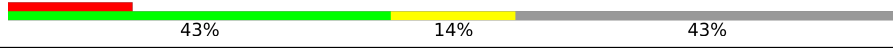
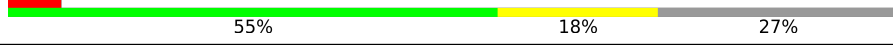
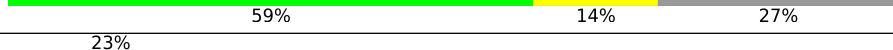
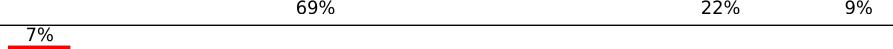
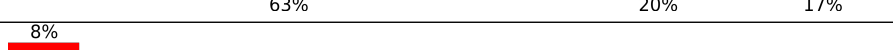
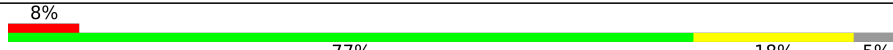
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1396	
1	G	1396	
1	M	1396	
1	N	1396	
1	O	1396	
1	P	1396	
1	Q	1396	
1	R	1396	
1	S	1396	
1	T	1396	
1	U	1396	
1	z	1396	
2	D	235	
2	H	235	
2	I	235	
2	J	235	
2	K	235	
2	L	235	
2	V	235	
2	W	235	
2	X	235	
2	Y	235	
2	Z	235	
2	a	235	
2	b	235	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	c	235	
2	d	235	
3	e	483	
3	f	483	
3	g	483	
3	h	483	
3	i	483	
4	j	316	
4	k	316	
4	l	316	
4	m	316	
4	n	316	
4	o	316	
4	p	316	
4	q	316	
4	r	316	
4	s	316	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 208346 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	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	M	1353	Total	C	N	O	S	0	0
			10582	6690	1876	1948	68		
1	N	1353	Total	C	N	O	S	0	0
			10582	6690	1876	1948	68		
1	O	1355	Total	C	N	O	S	0	0
			10600	6701	1881	1950	68		
1	P	1355	Total	C	N	O	S	0	0
			10600	6701	1881	1950	68		
1	Q	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	R	1353	Total	C	N	O	S	0	0
			10582	6690	1876	1948	68		
1	S	1355	Total	C	N	O	S	0	0
			10600	6701	1881	1950	68		
1	T	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	U	1331	Total	C	N	O	S	0	0
			10422	6590	1847	1919	66		
1	B	1355	Total	C	N	O	S	0	0
			10600	6701	1881	1950	68		
1	C	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	E	1353	Total	C	N	O	S	0	0
			10582	6689	1877	1948	68		
1	F	1354	Total	C	N	O	S	0	0
			10592	6695	1880	1949	68		
1	G	1295	Total	C	N	O	S	0	0
			10133	6401	1804	1863	65		
1	z	607	Total	C	N	O	S	0	0
			4709	2970	830	878	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	V	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	W	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	X	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	Y	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	Z	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	a	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	b	99	Total	C	N	O	S	0	0
			754	475	142	135	2		
2	c	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	d	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	H	99	Total	C	N	O	S	0	0
			754	475	142	135	2		
2	I	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	J	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	K	100	Total	C	N	O	S	0	0
			765	481	146	136	2		
2	L	100	Total	C	N	O	S	0	0
			765	481	146	136	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	275	Total	C	N	O	S	0	0
			2194	1394	392	393	15		
3	f	351	Total	C	N	O	S	0	0
			2768	1746	499	507	16		
3	g	307	Total	C	N	O	S	0	0
			2419	1526	434	444	15		
3	h	340	Total	C	N	O	S	0	0
			2688	1695	485	492	16		
3	i	353	Total	C	N	O	S	0	0
			2789	1760	501	512	16		

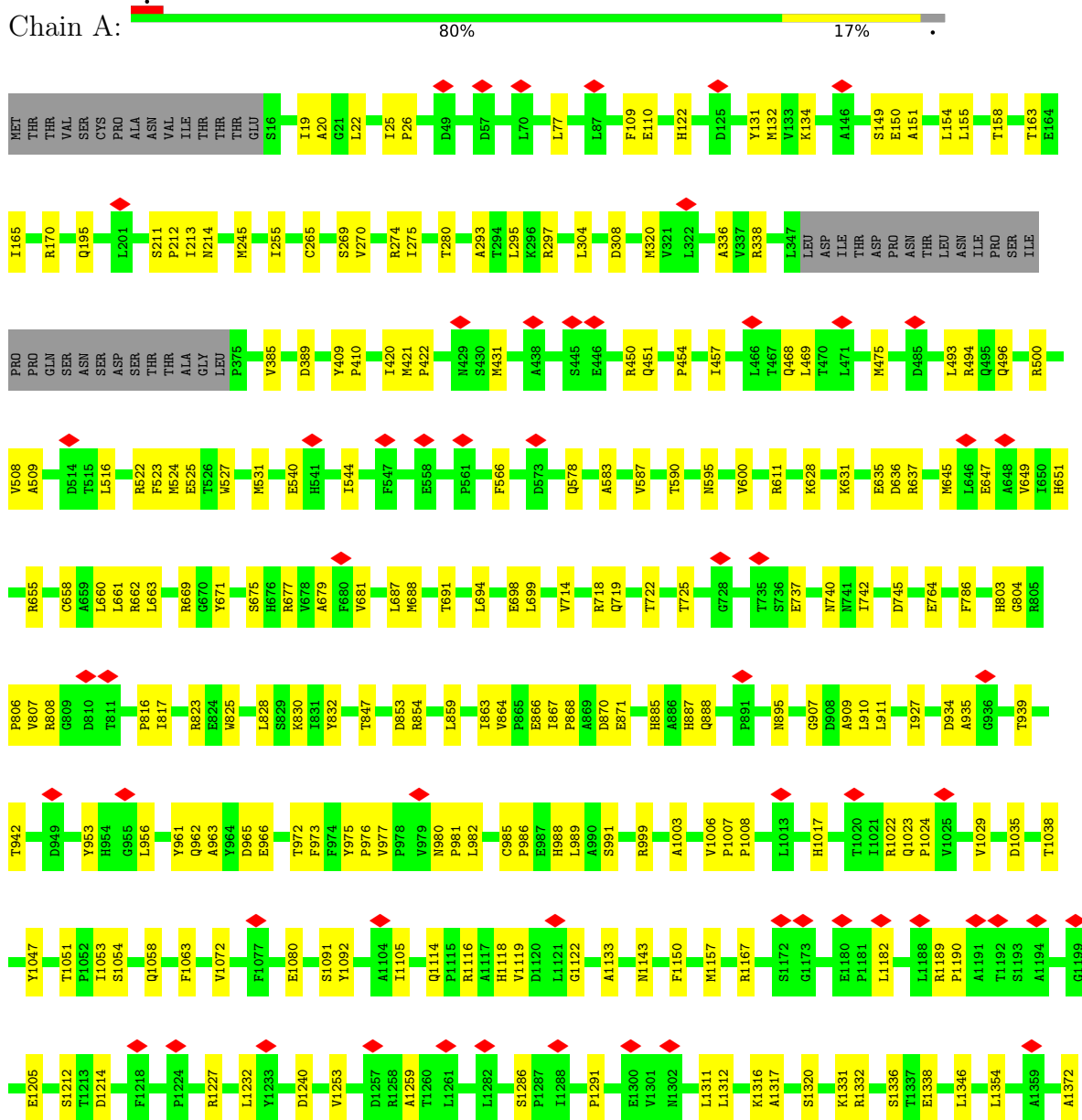
- Molecule 4 is a protein called Triplex capsid protein 2.

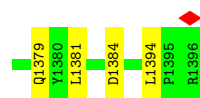
Mol	Chain	Residues	Atoms					AltConf	Trace
4	j	241	Total	C	N	O	S	0	0
			1837	1180	310	337	10		
4	o	258	Total	C	N	O	S	0	0
			1969	1259	334	366	10		
4	k	289	Total	C	N	O	S	0	0
			2199	1401	378	410	10		
4	p	301	Total	C	N	O	S	0	0
			2307	1470	400	424	13		
4	l	262	Total	C	N	O	S	0	0
			2005	1283	341	371	10		
4	q	254	Total	C	N	O	S	0	0
			1937	1235	330	362	10		
4	m	276	Total	C	N	O	S	0	0
			2105	1346	361	388	10		
4	r	301	Total	C	N	O	S	0	0
			2307	1469	400	426	12		
4	n	276	Total	C	N	O	S	0	0
			2105	1346	361	388	10		
4	s	302	Total	C	N	O	S	0	0
			2312	1472	401	427	12		

3 Residue-property plots

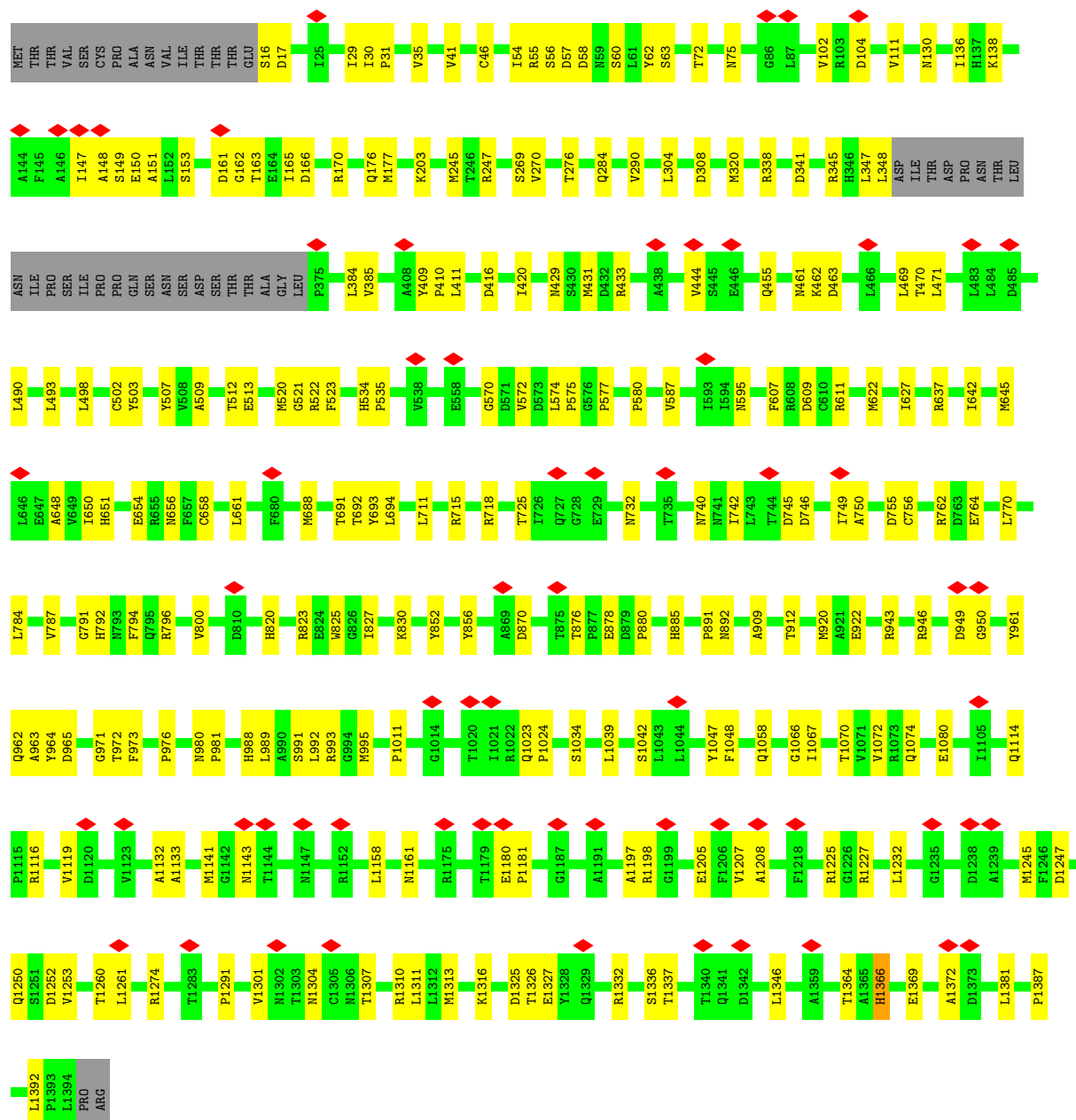
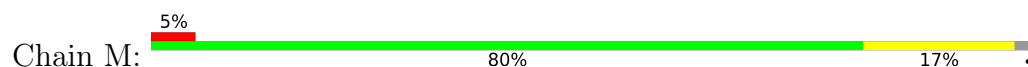
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Major capsid protein

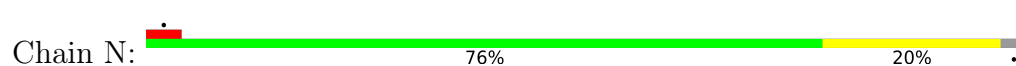


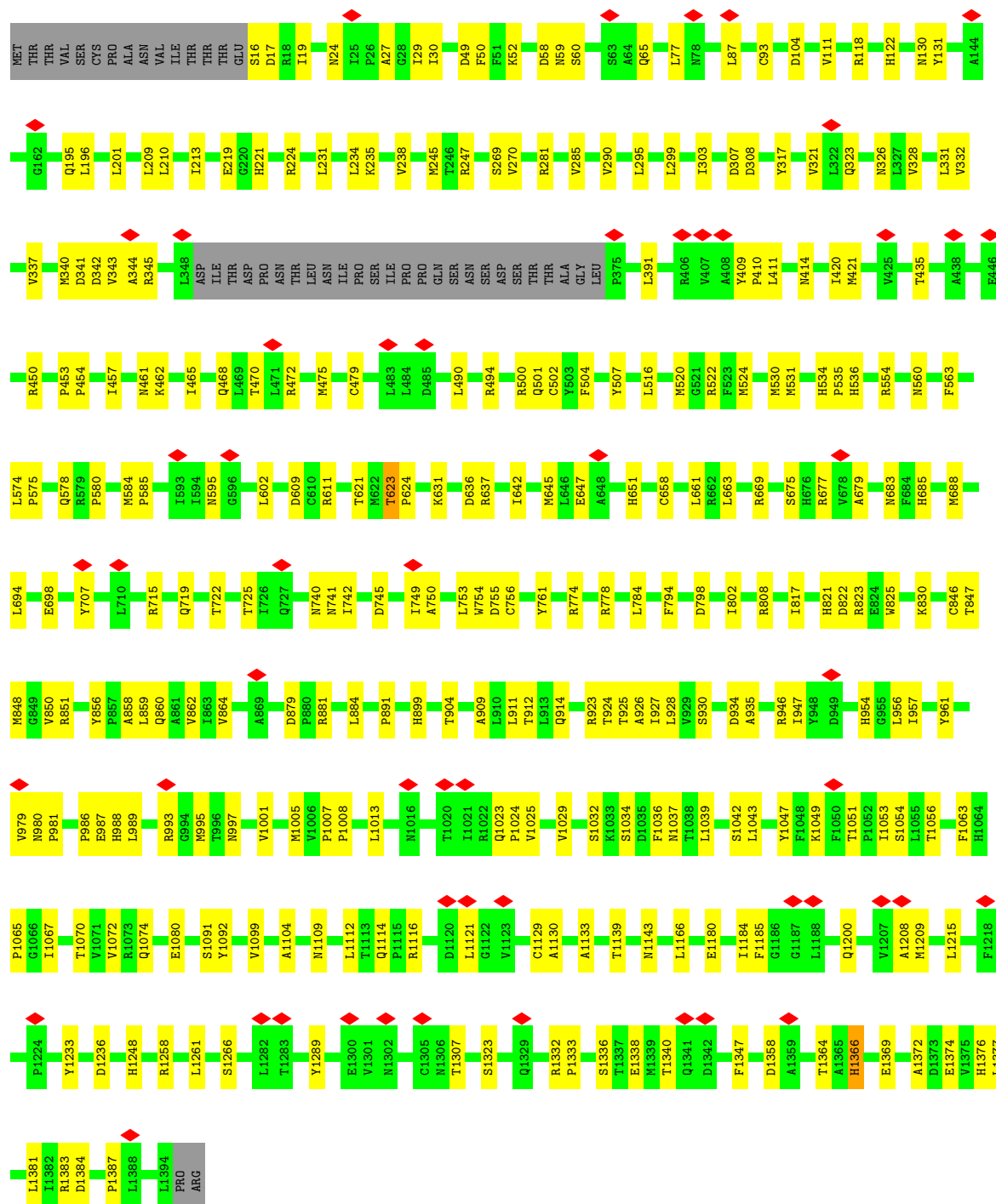


• Molecule 1: Major capsid protein



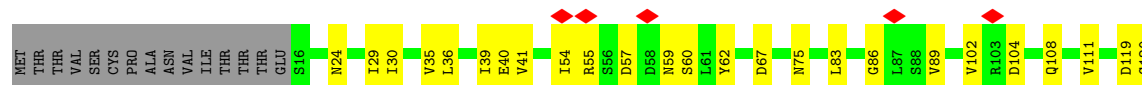
• Molecule 1: Major capsid protein

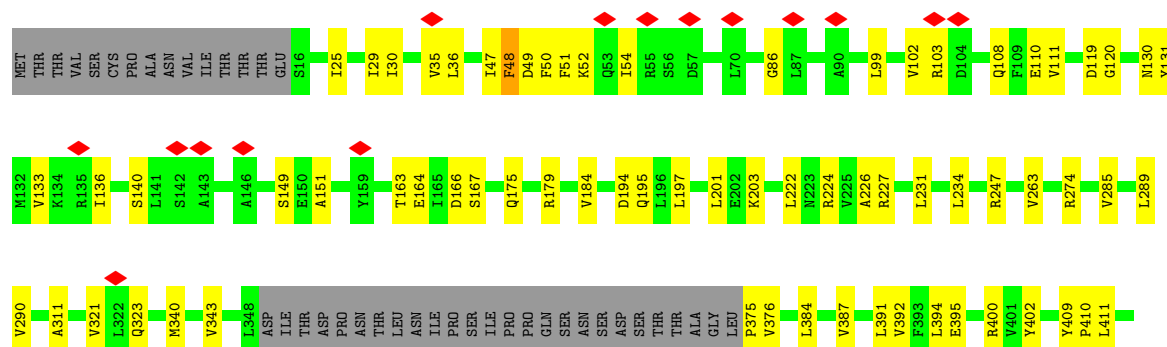
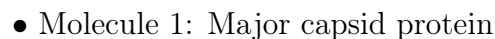


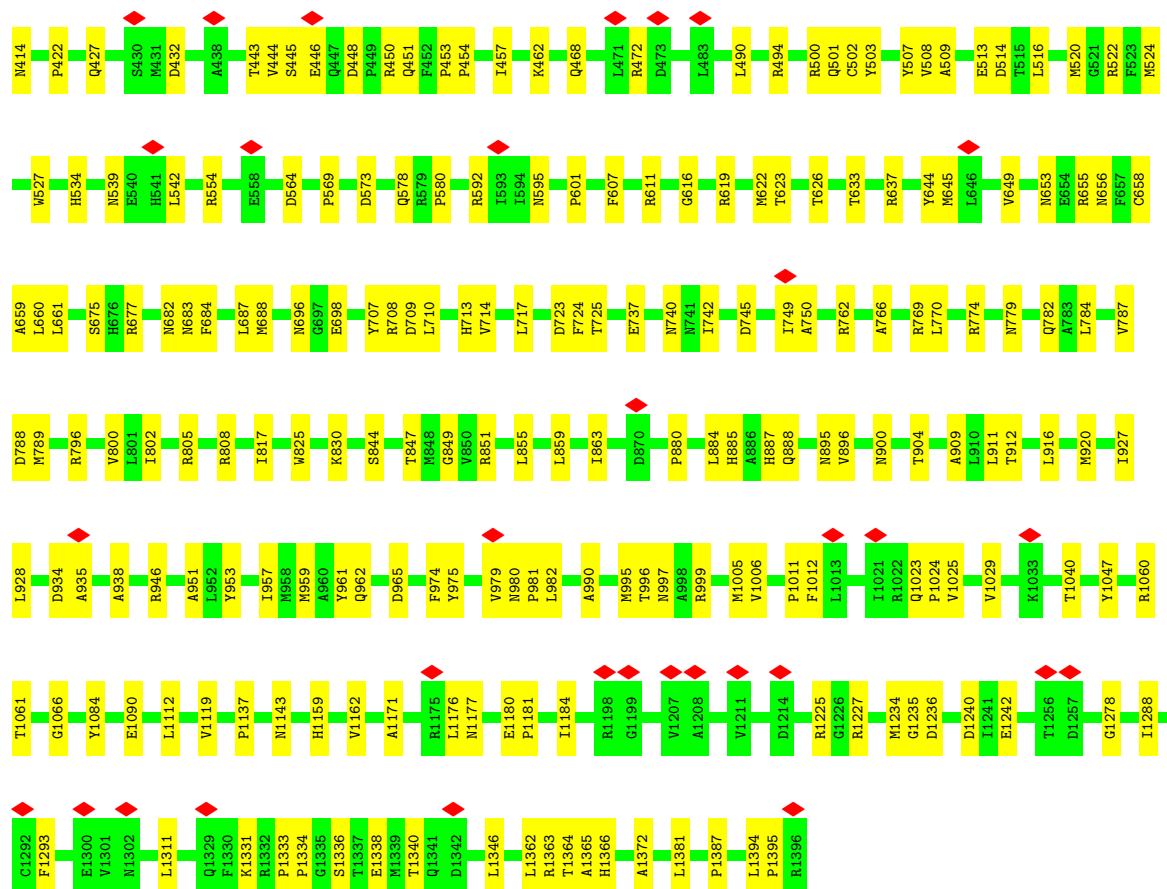


• Molecule 1: Major capsid protein

Chain O: 78% 19%

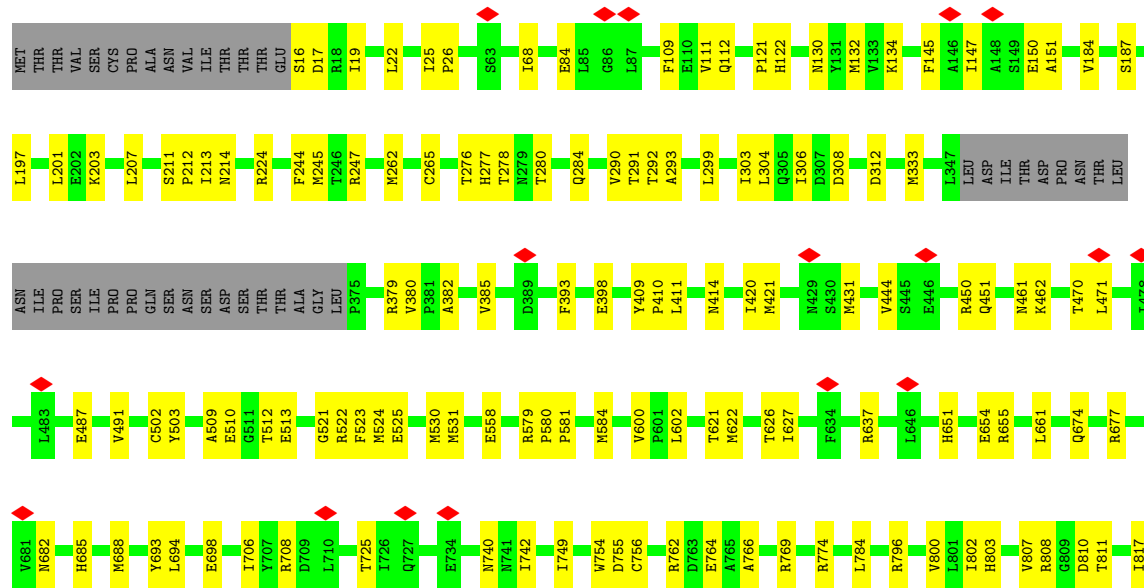


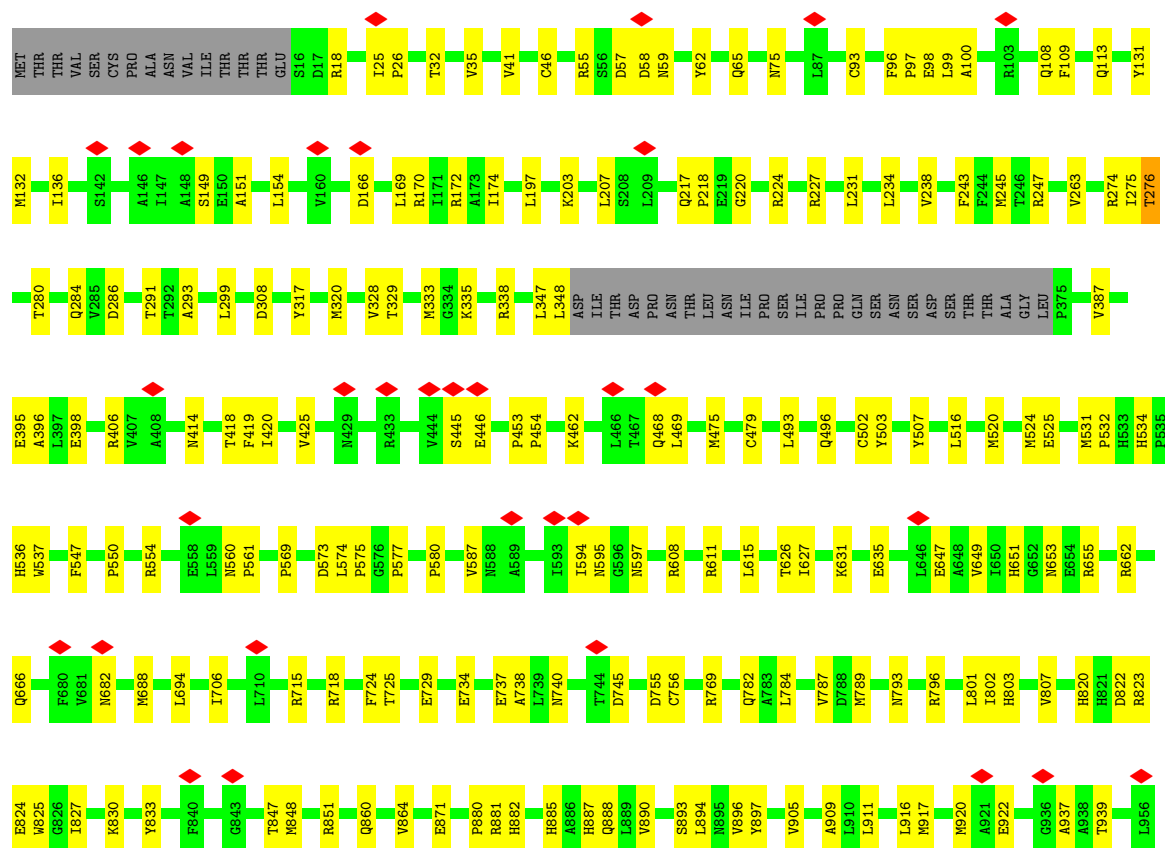


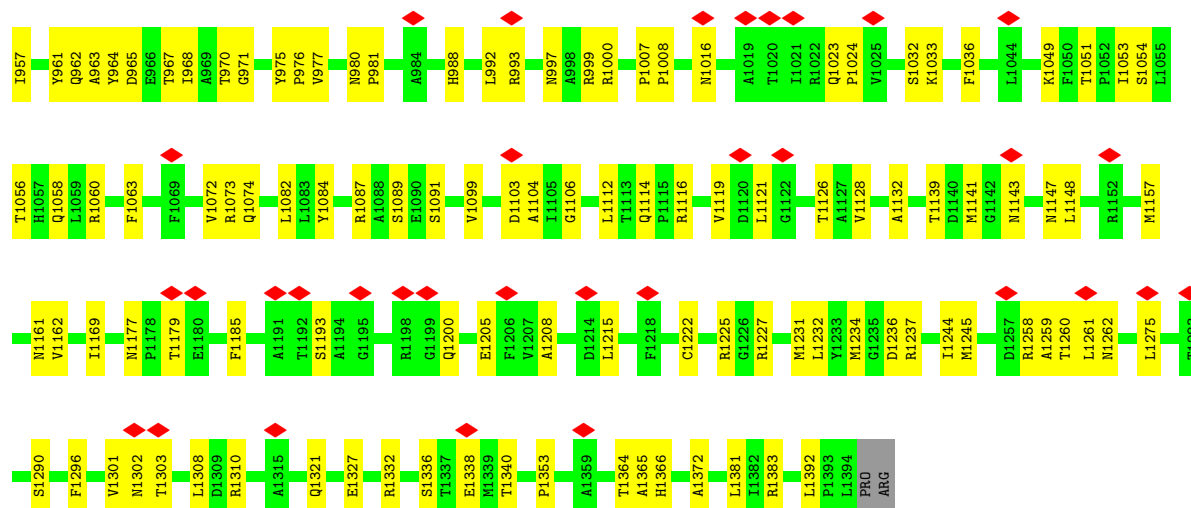


• Molecule 1: Major capsid protein

Chain Q:

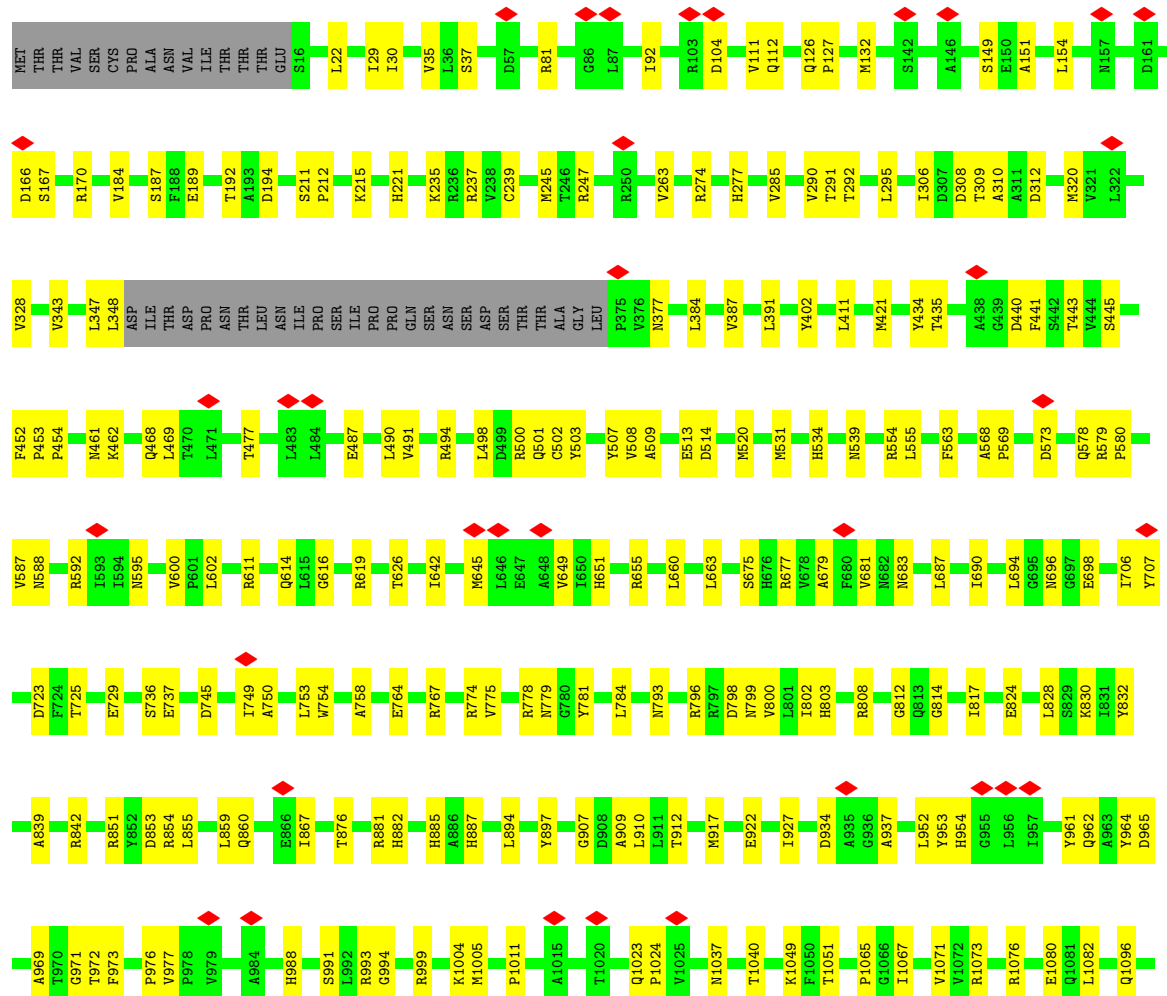


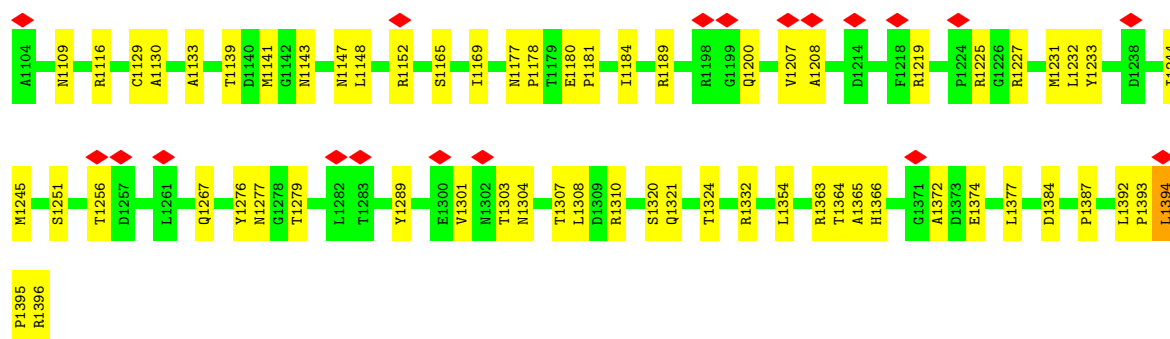




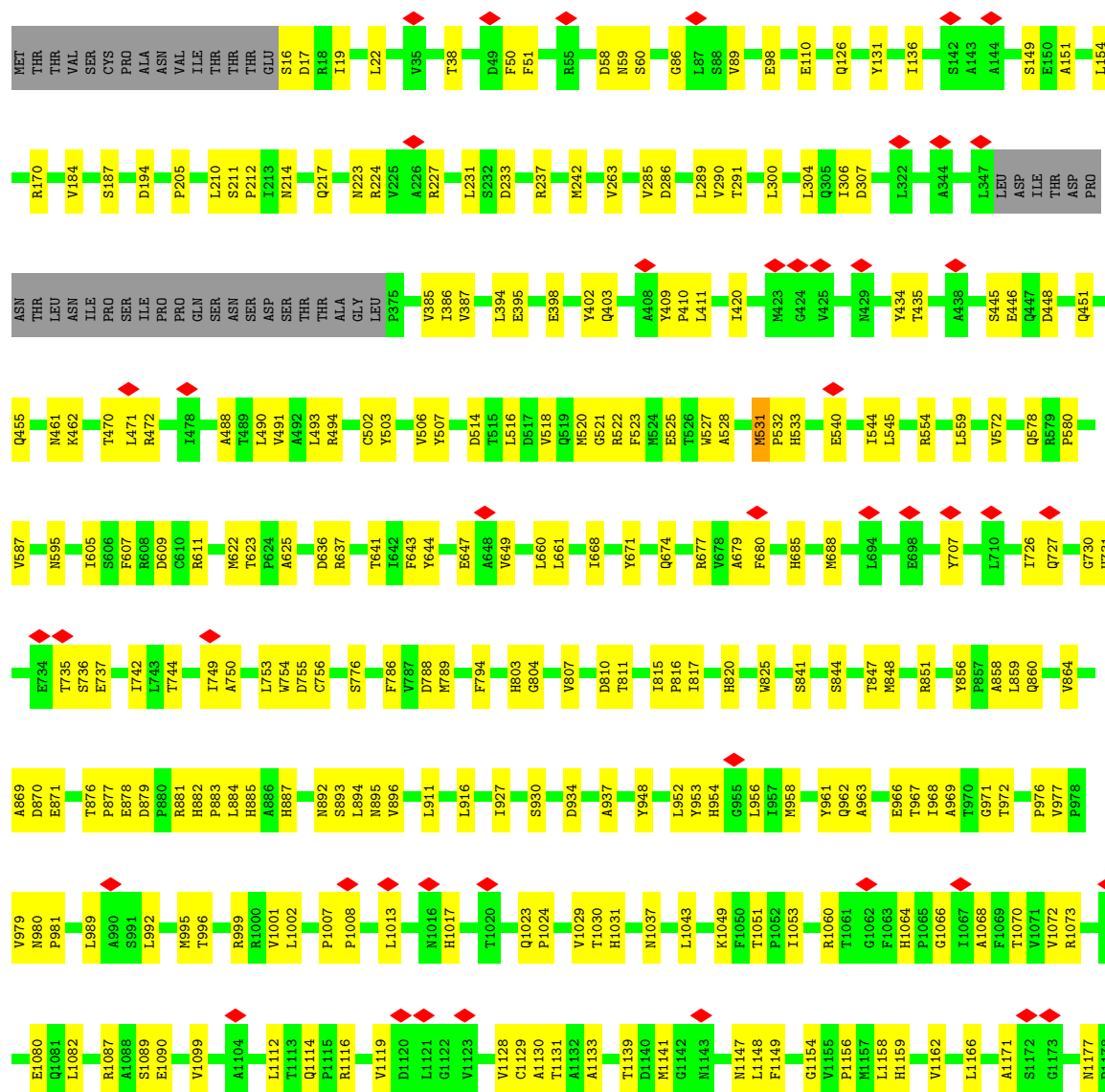
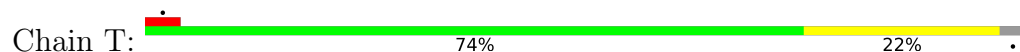
• Molecule 1: Major capsid protein

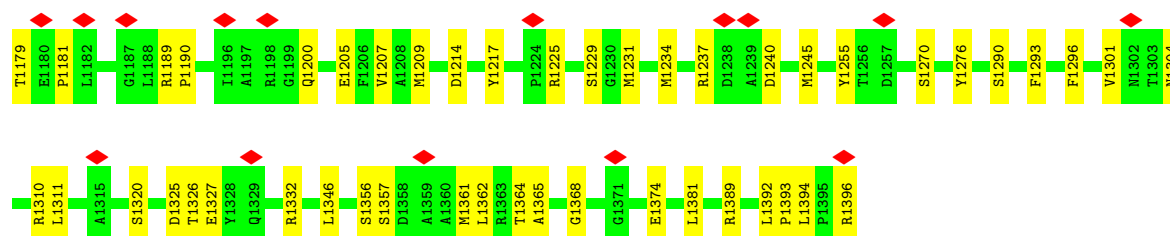
Chain S: 77% 20%



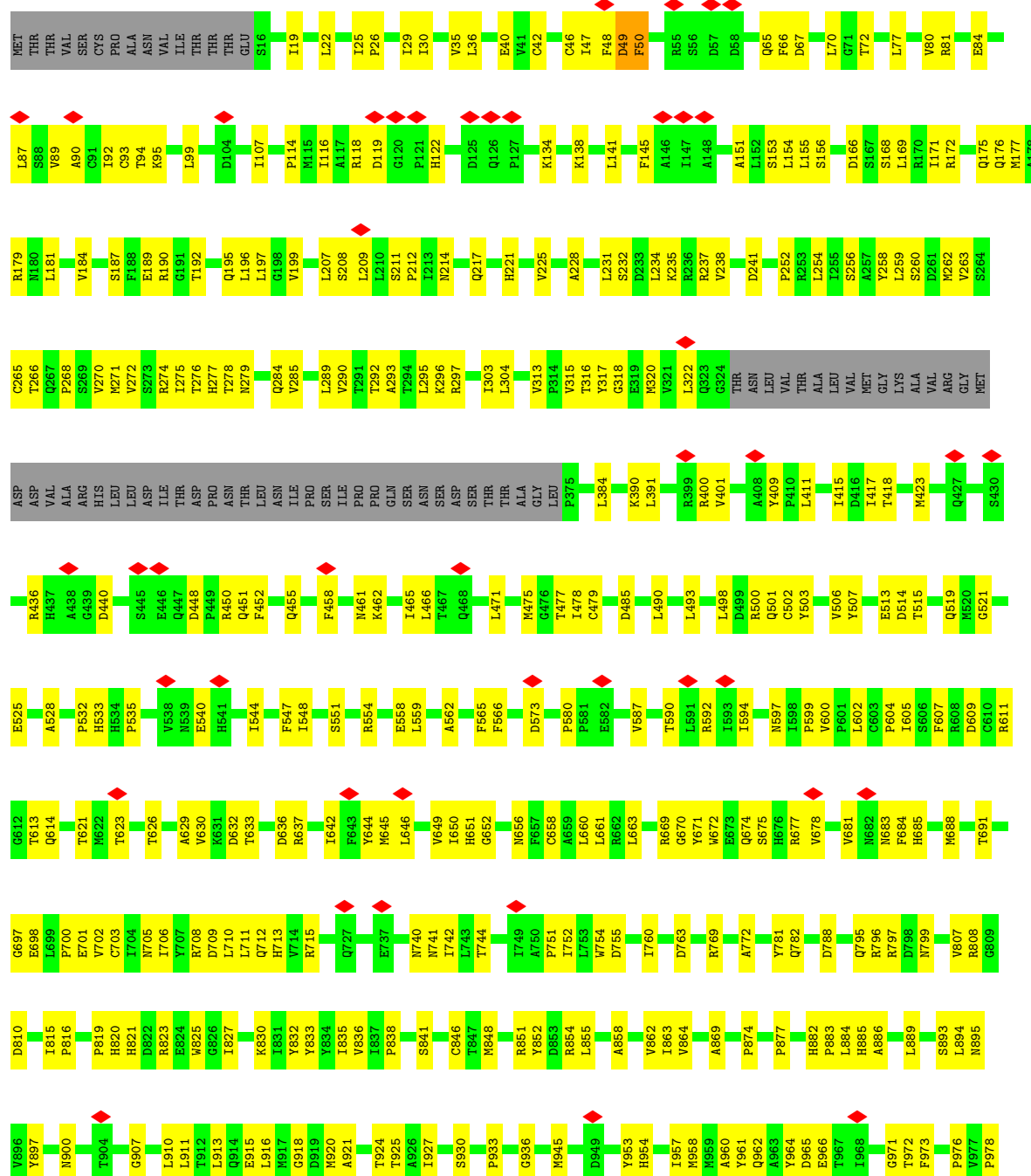


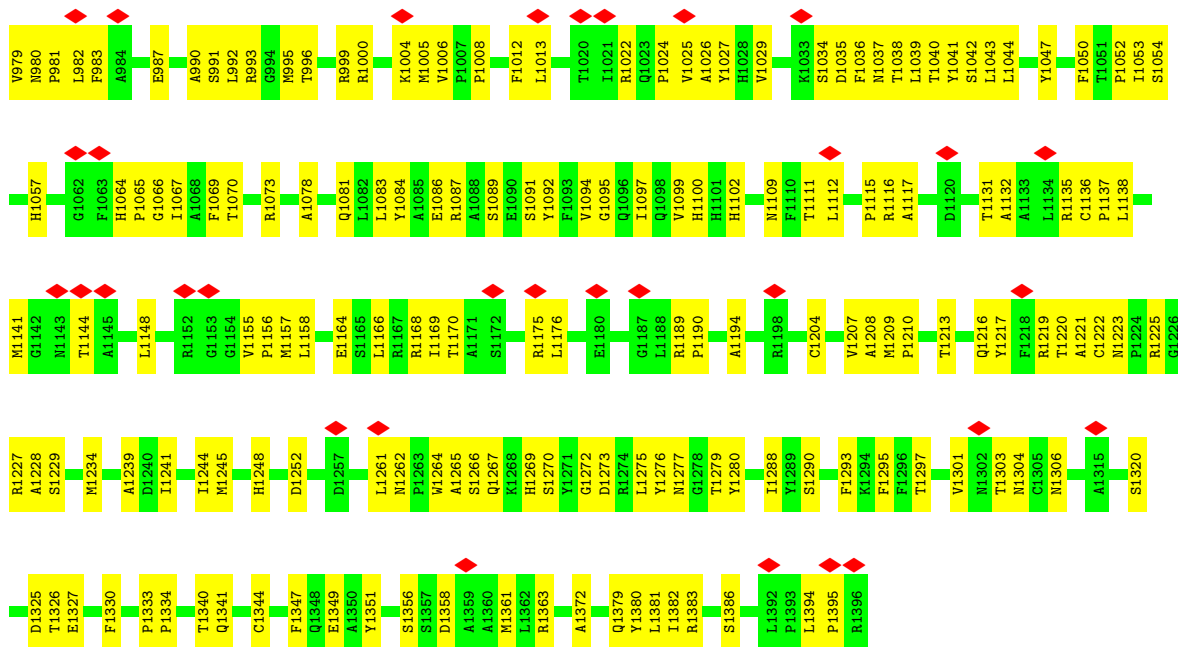
• Molecule 1: Major capsid protein

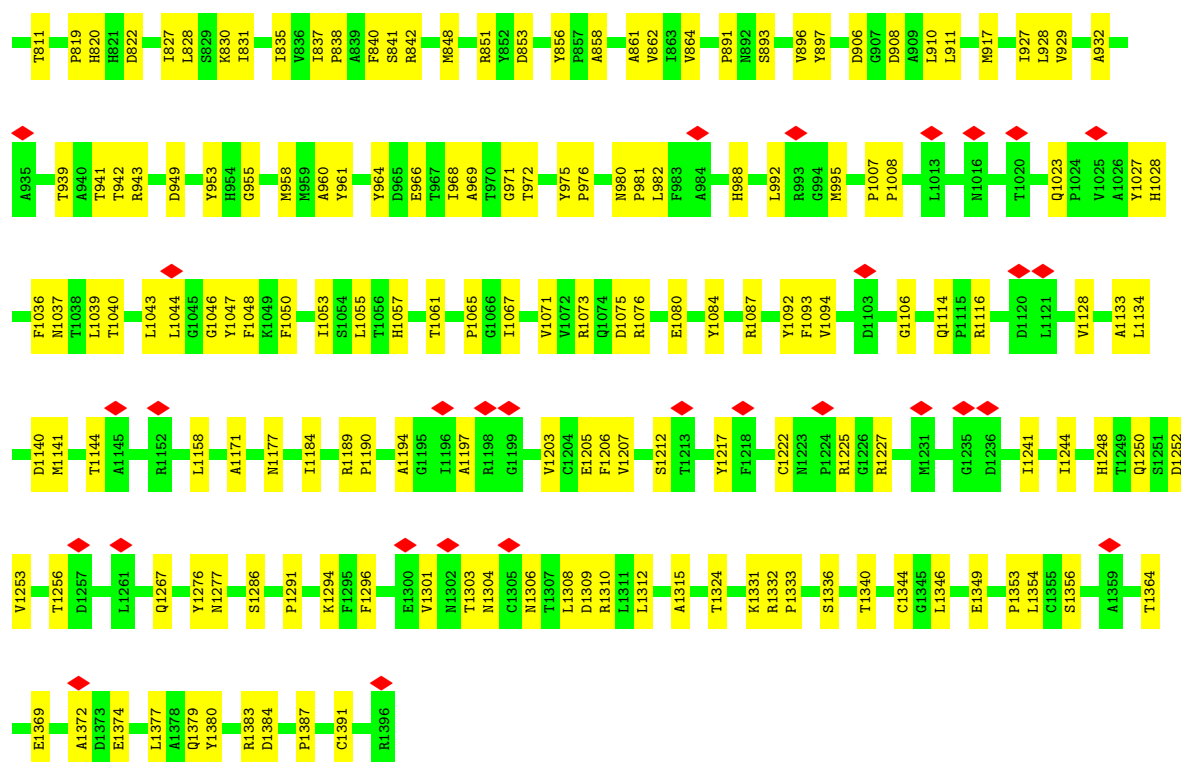




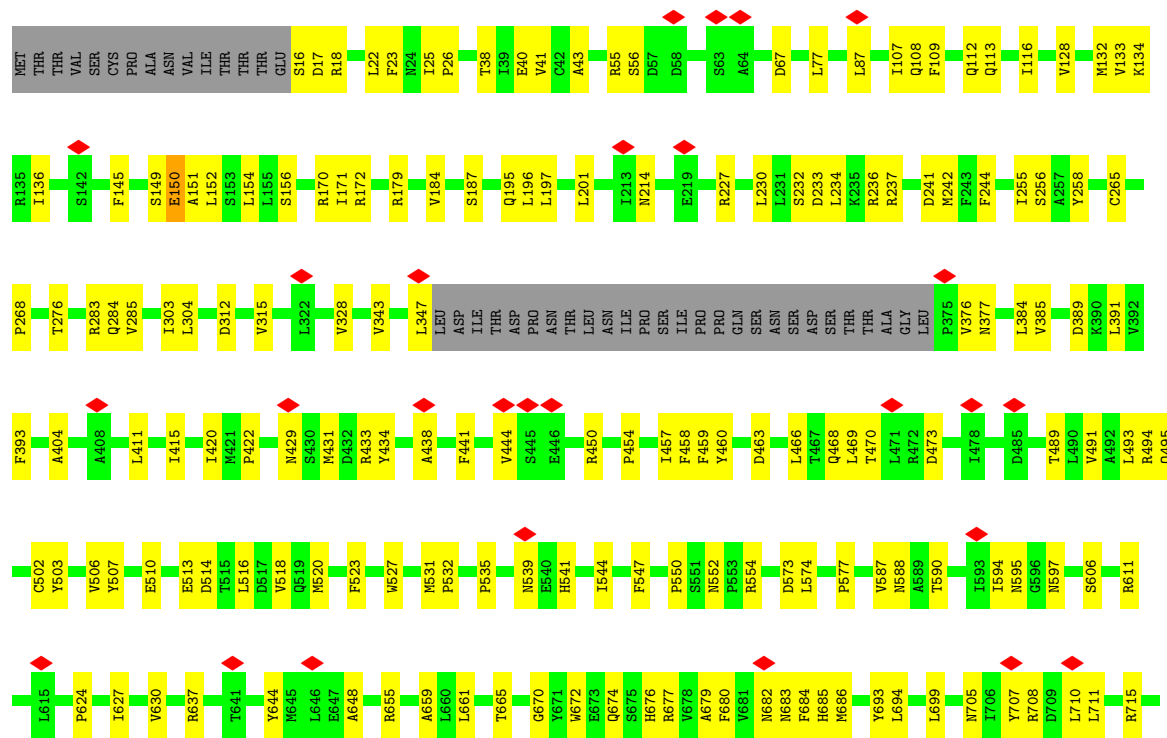
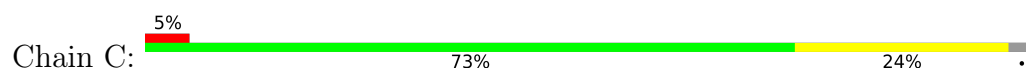
• Molecule 1: Major capsid protein

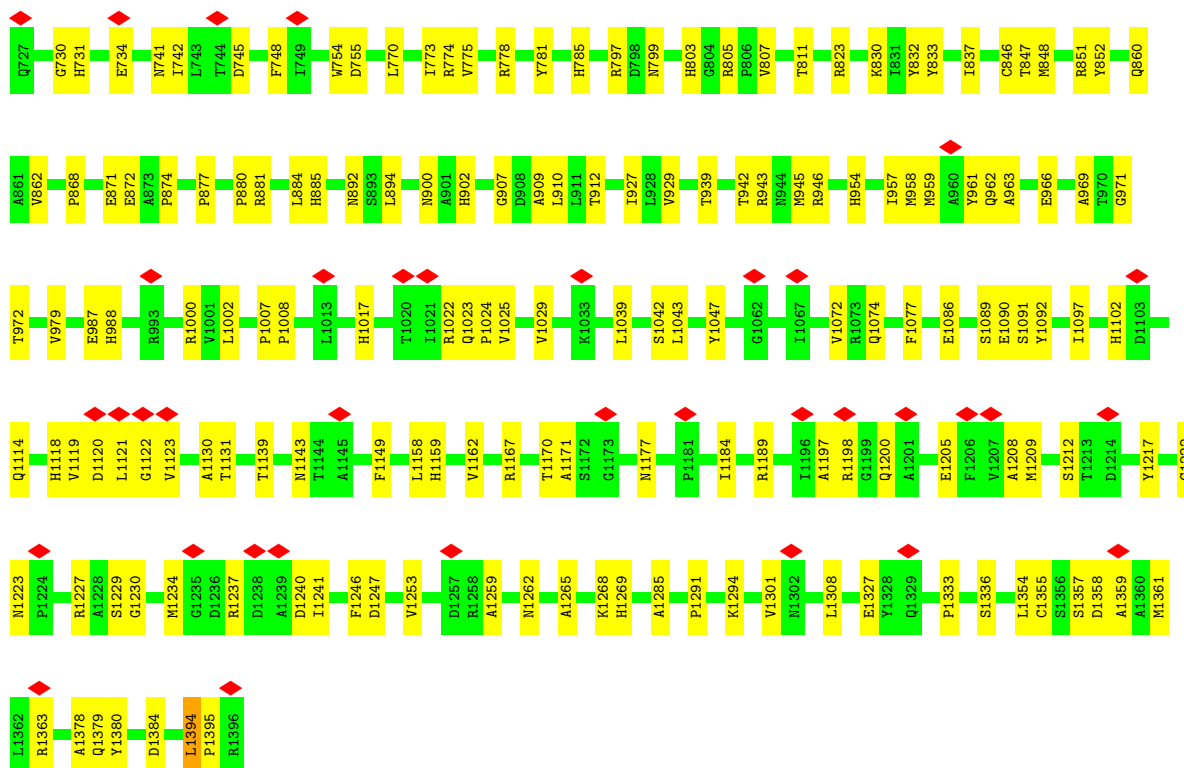




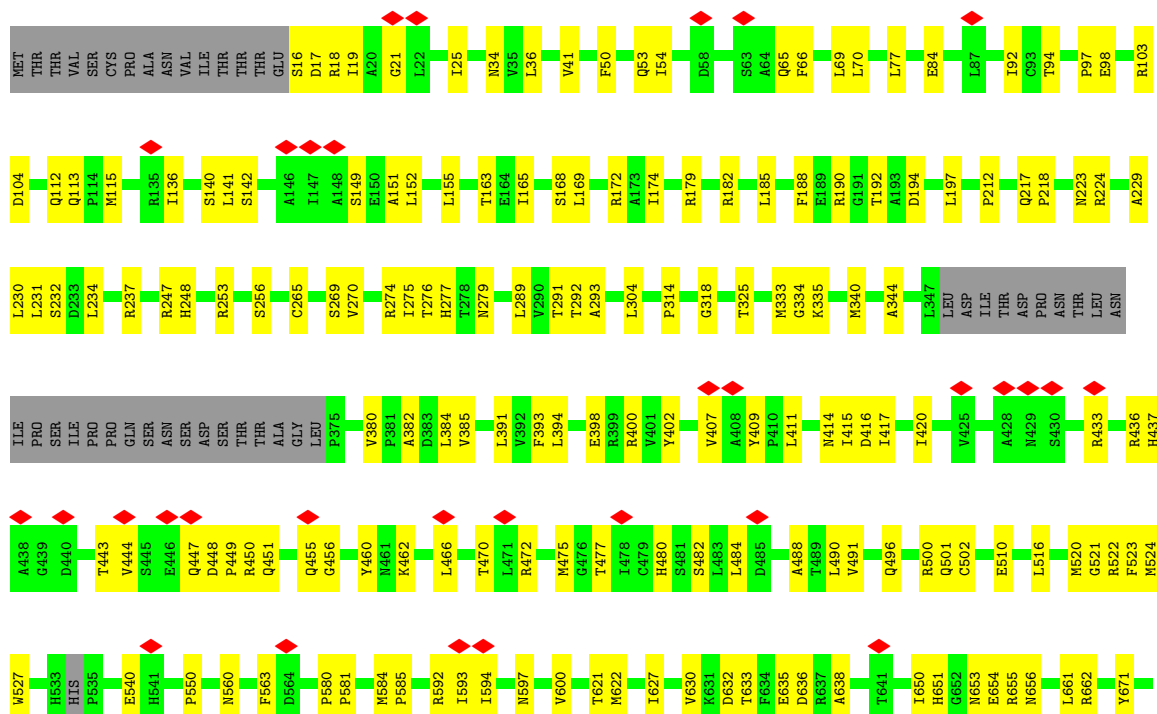


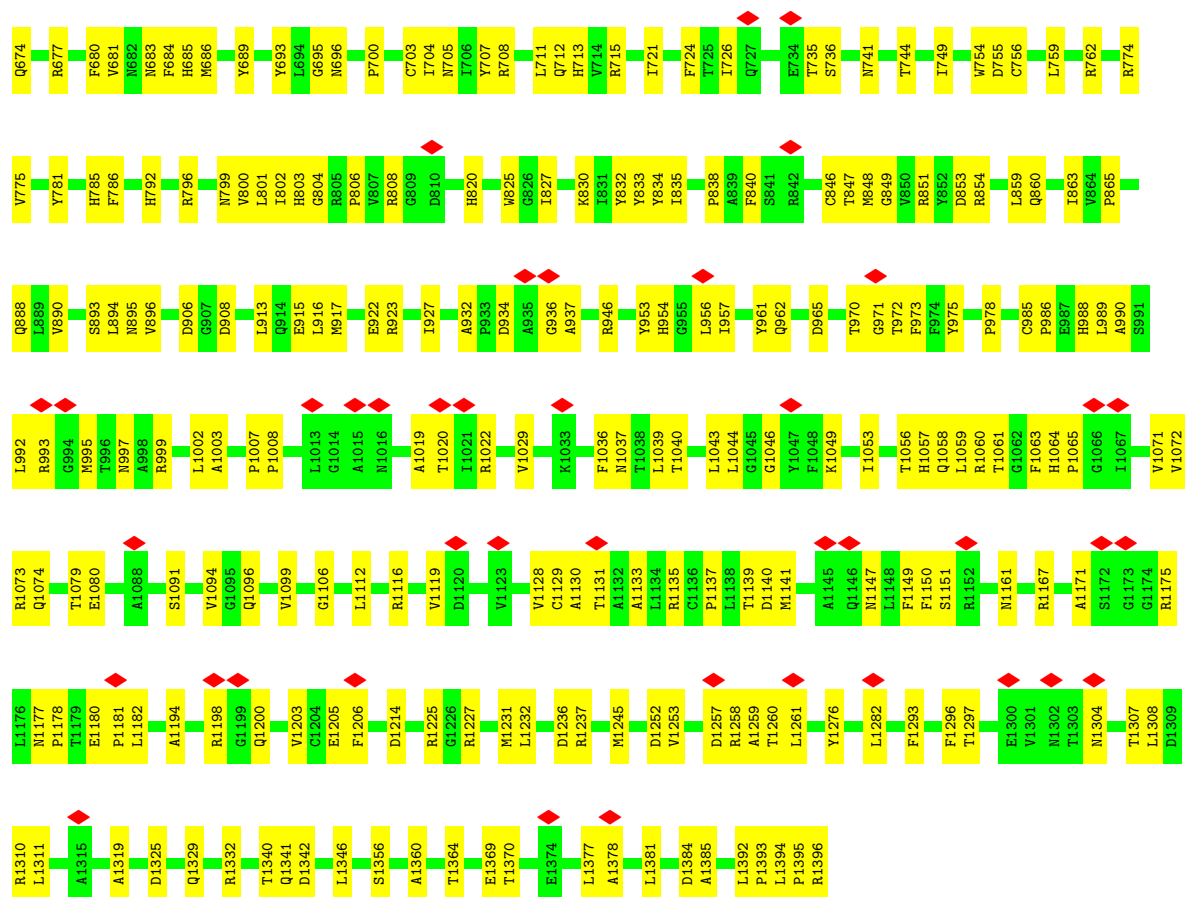
• Molecule 1: Major capsid protein



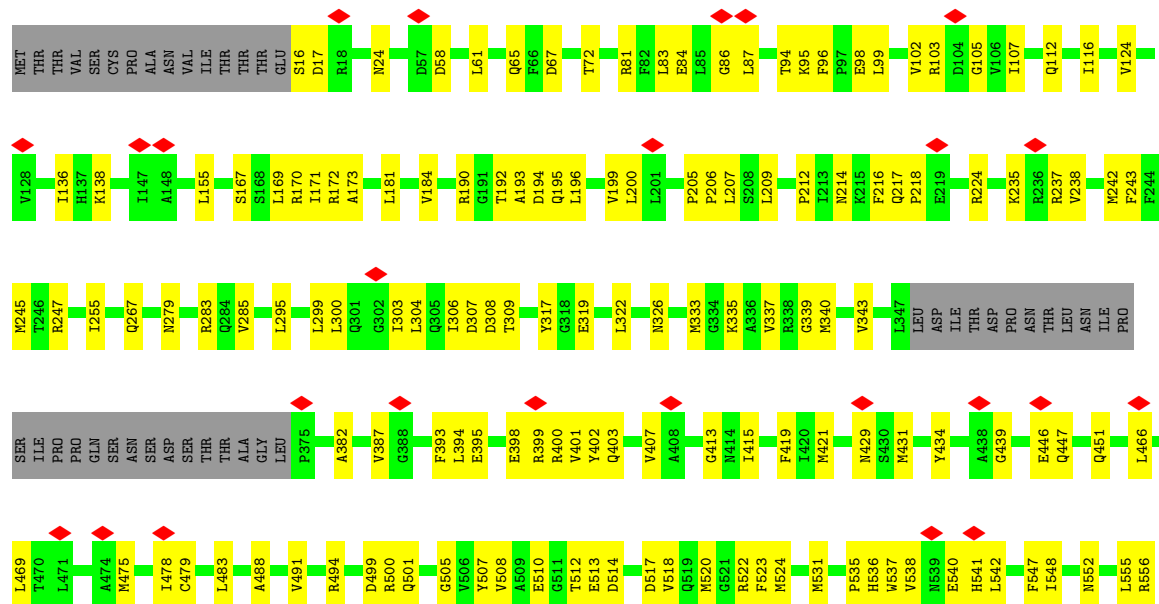


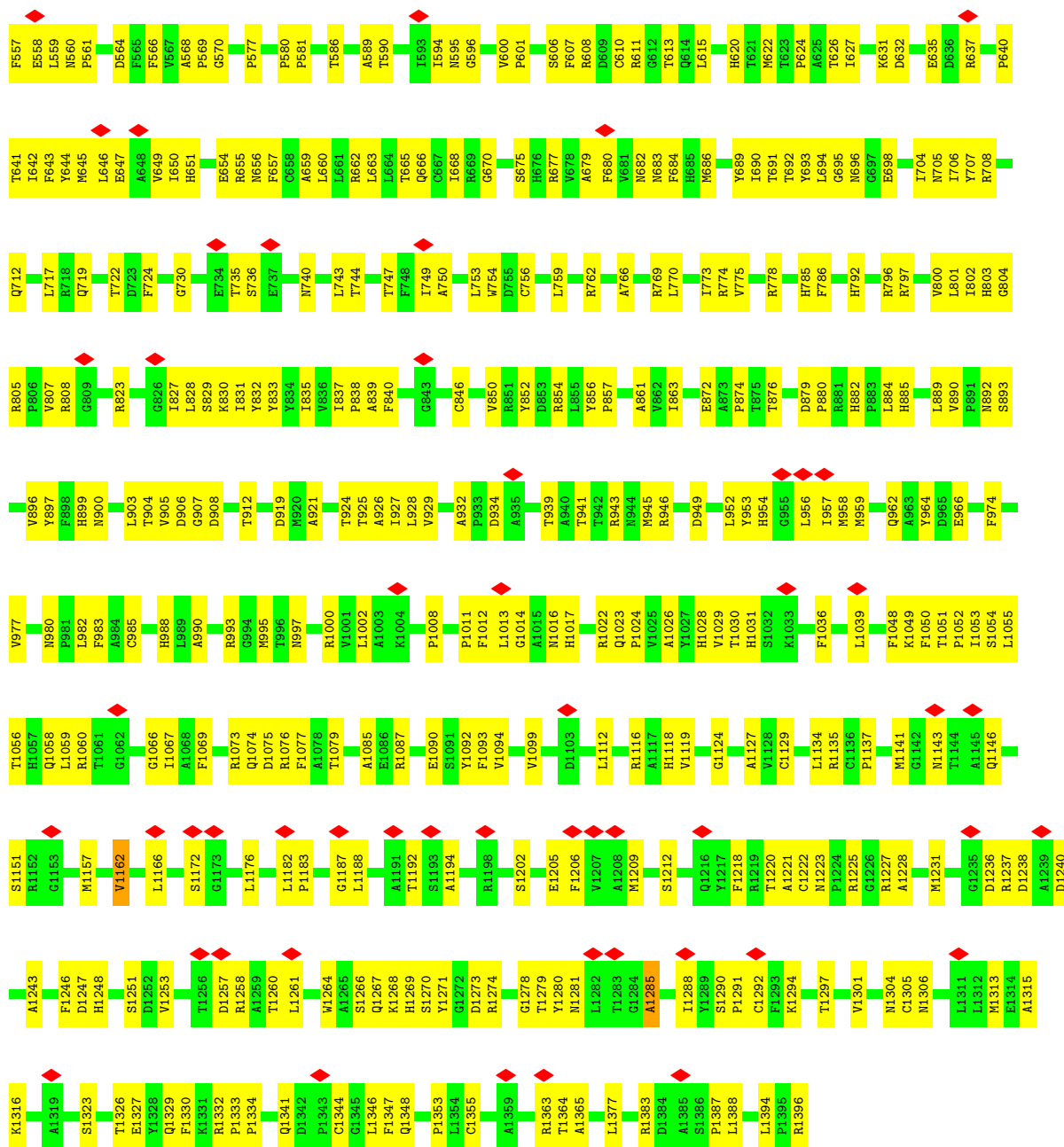
• Molecule 1: Major capsid protein





• Molecule 1: Major capsid protein

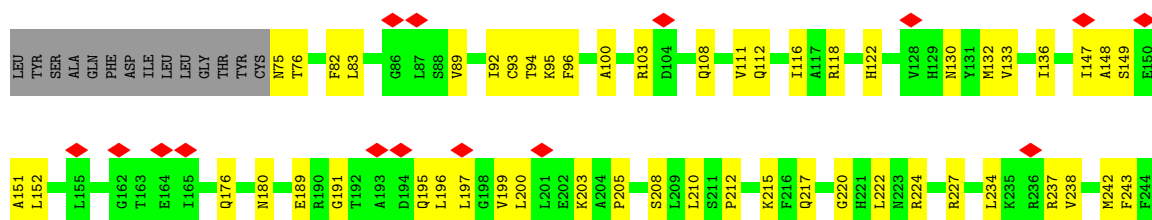




• Molecule 1: Major capsid protein



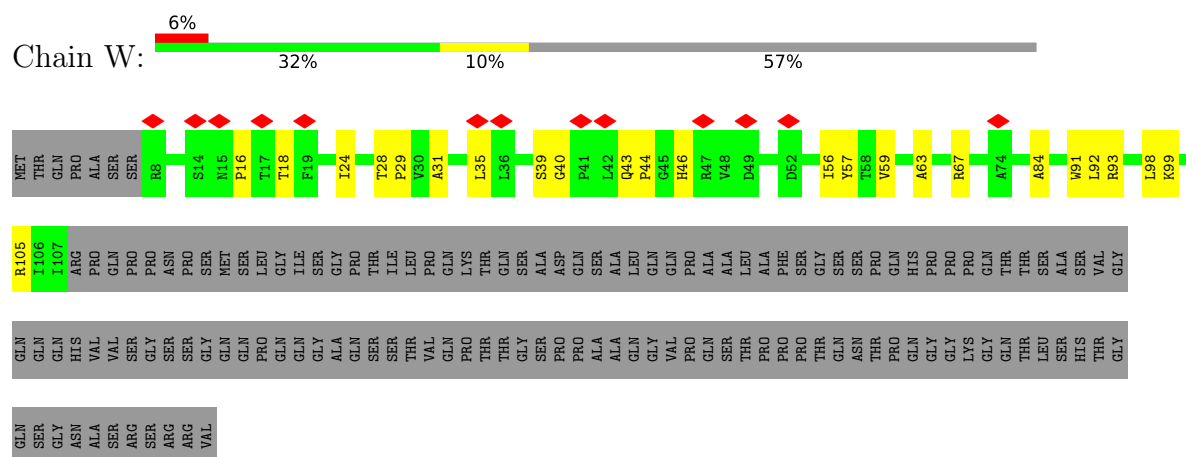
MET	THR	THR	VAL	SER	CYS	PRO	ALA	ASN	VAL	ILE	THR	THR	THR	GLU	SER	ASP	ARG	ILE	ALA	GLY	LEU	PHE	ASN	ILE	PRO	ALA	GLY	ASN	VAL	LEU	SER	THR	ILE	GLU	VAL	CYS	ALA	HIS	ARG	CYS	ILE	PHE	ASP	PHE	PHE	LYS	GLN	ILE	ARG	SER	ASP	ASN	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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



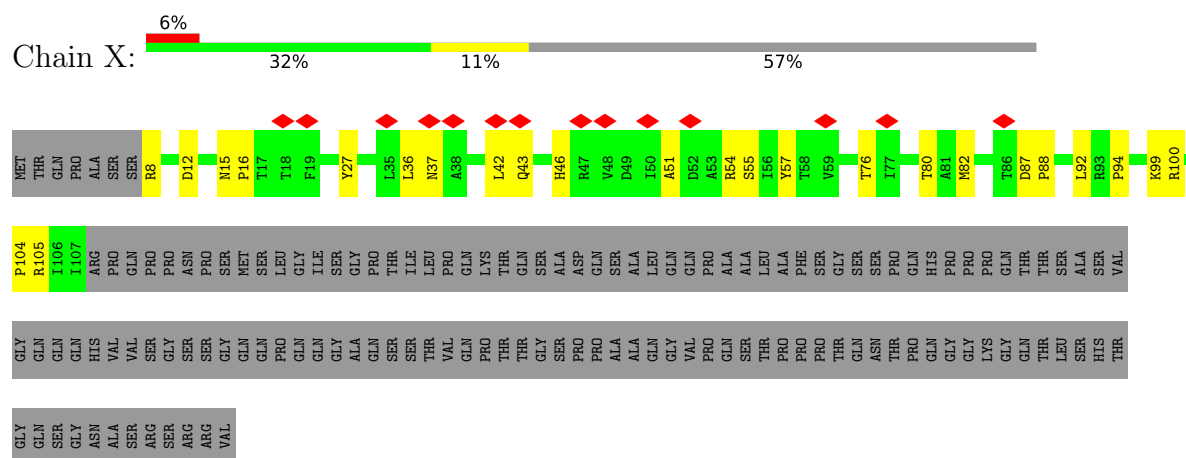




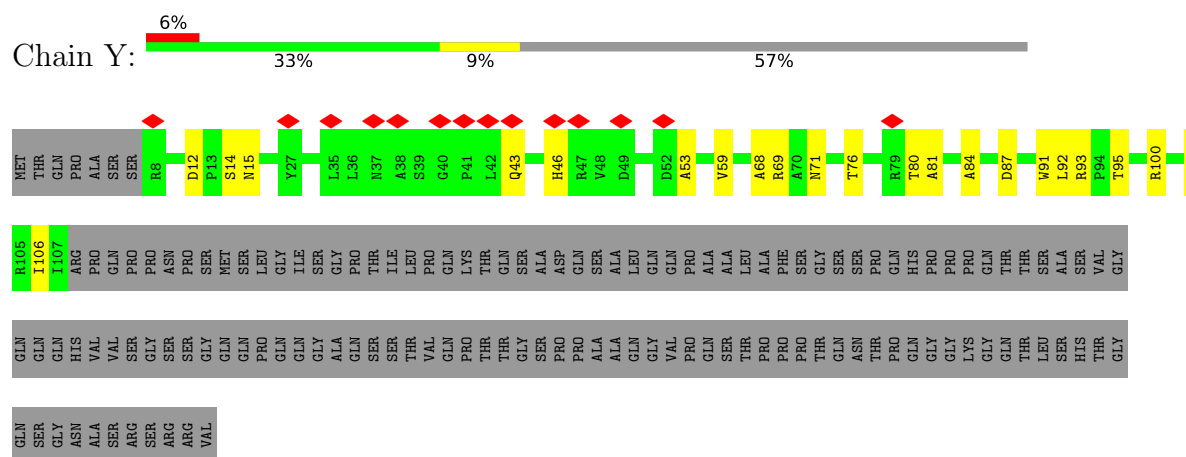
- Molecule 2: Small capsomere-interacting protein



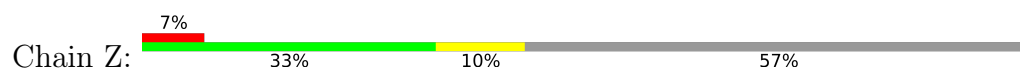
- Molecule 2: Small capsomere-interacting protein

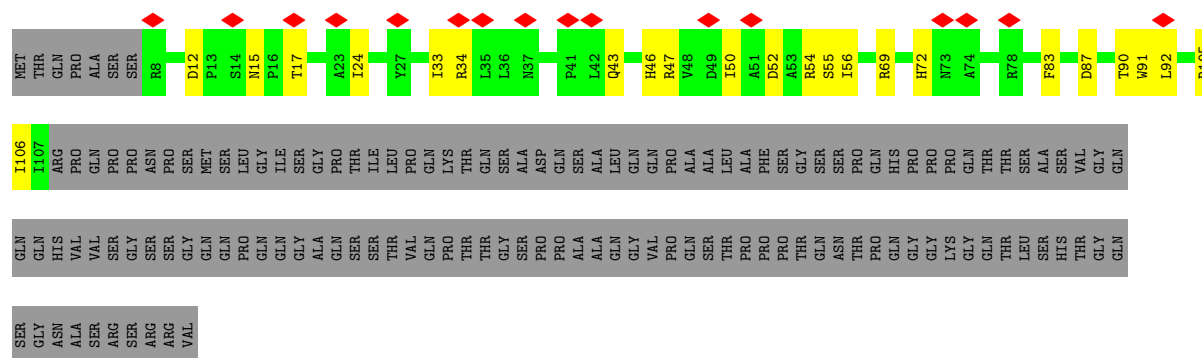


- Molecule 2: Small capsomere-interacting protein

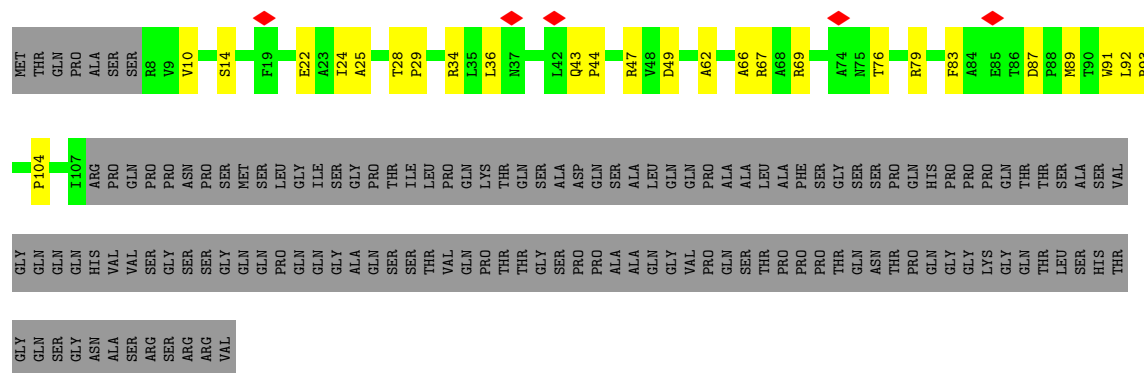
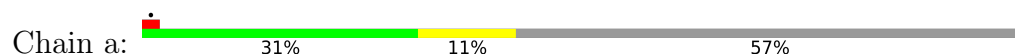


- Molecule 2: Small capsomere-interacting protein

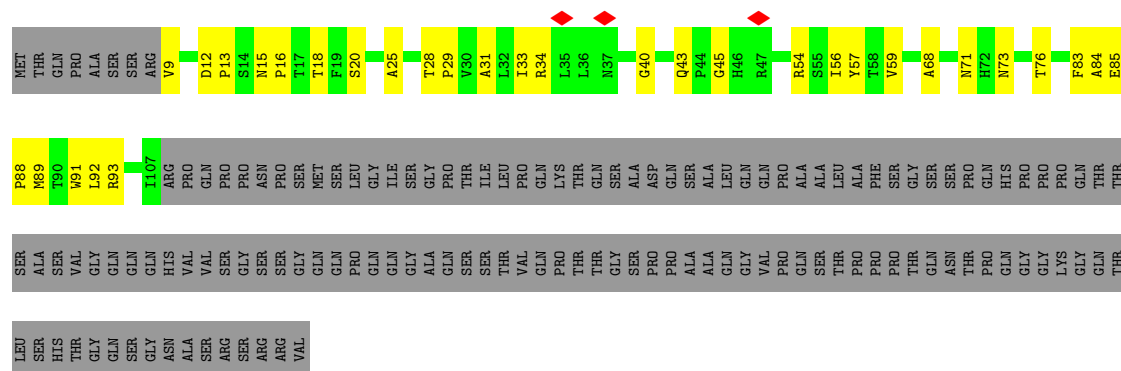




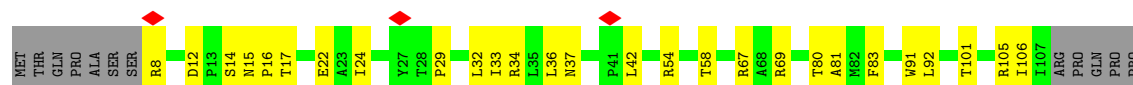
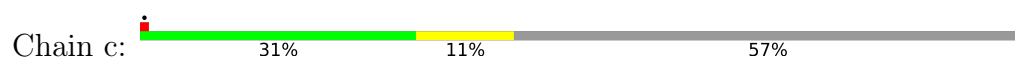
• Molecule 2: Small capsomere-interacting protein



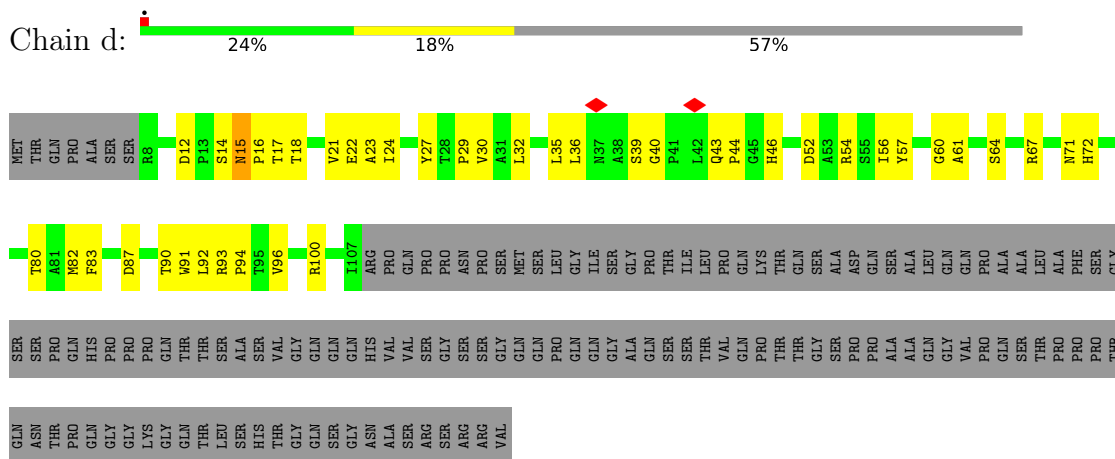
• Molecule 2: Small capsomere-interacting protein



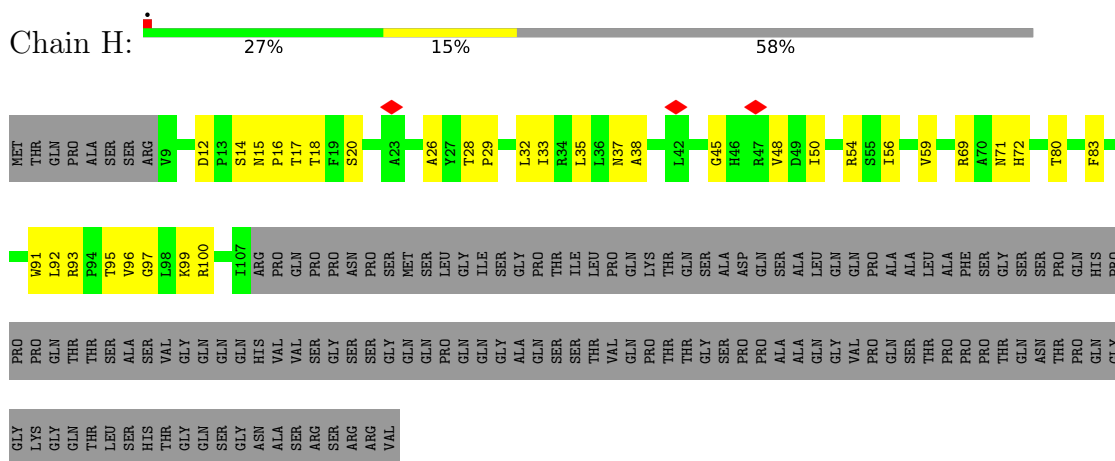
• Molecule 2: Small capsomere-interacting protein



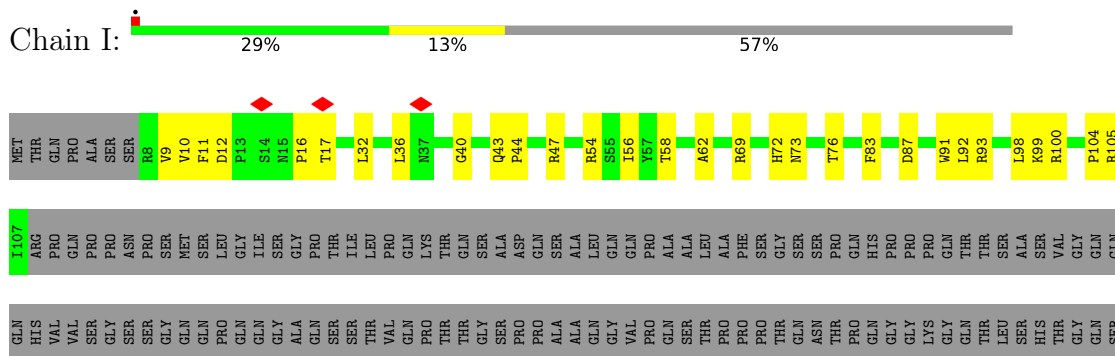
- Molecule 2: Small capsomere-interacting protein

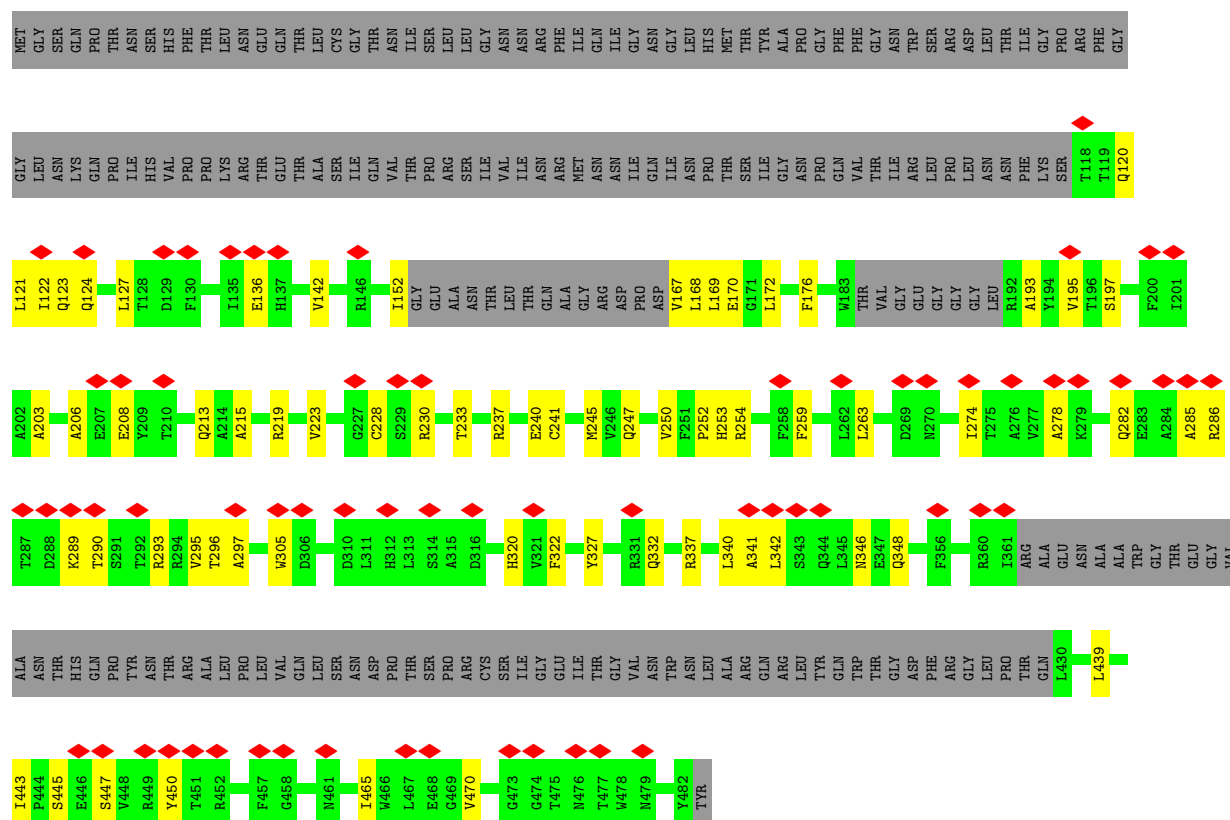
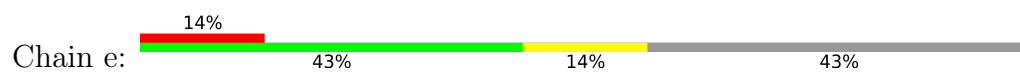


- Molecule 2: Small capsomere-interacting protein

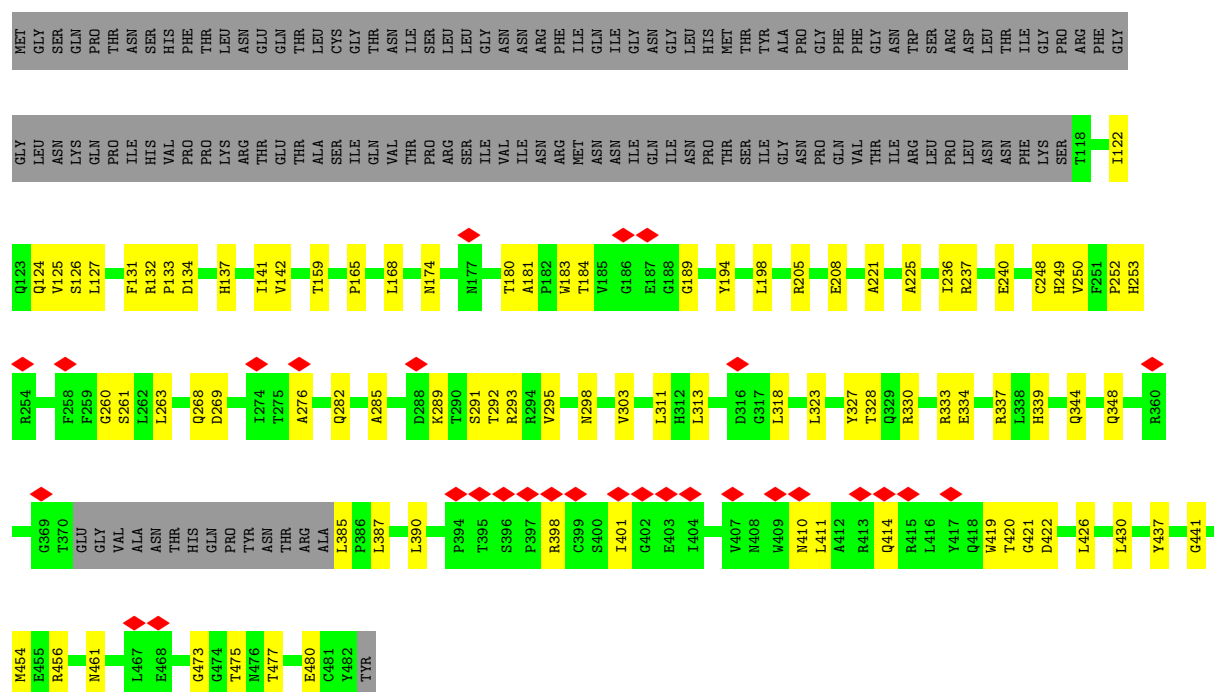


- Molecule 2: Small capsomere-interacting protein

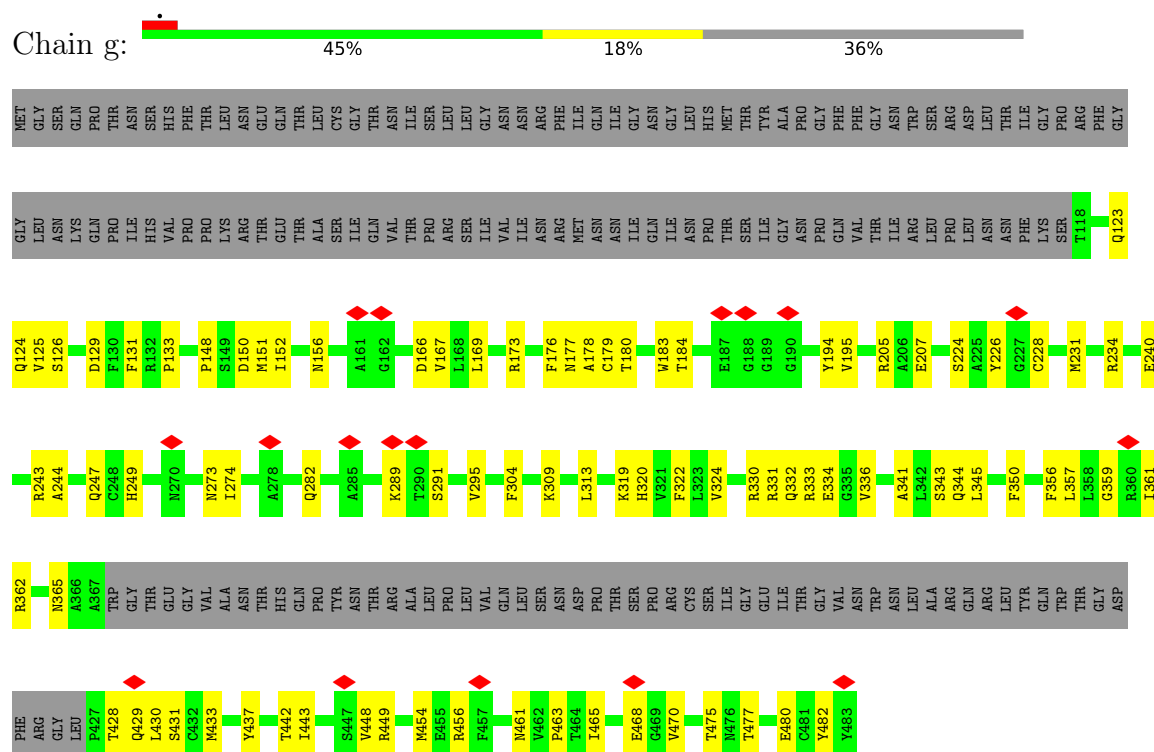




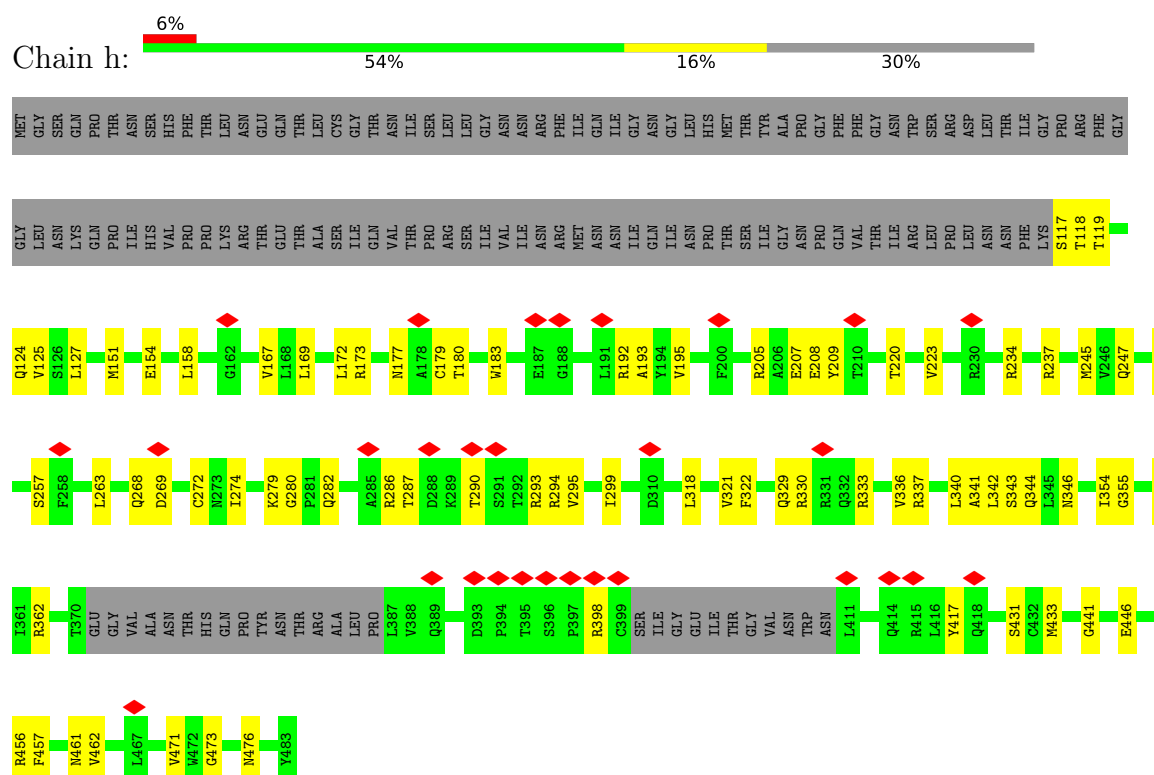
• Molecule 3: Triplex capsid protein 1



- Molecule 3: Triplex capsid protein 1



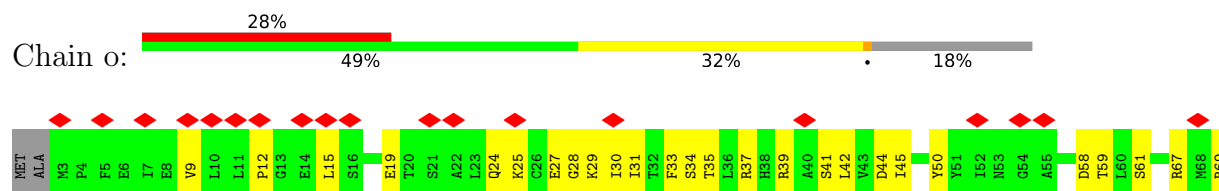
- Molecule 3: Triplex capsid protein 1

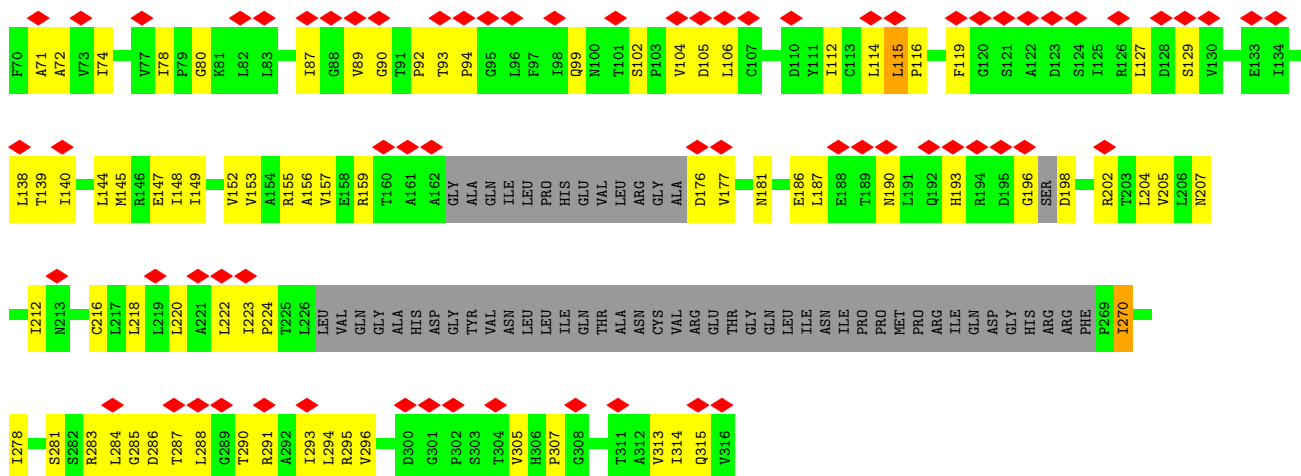


- Molecule 3: Triplex capsid protein 1

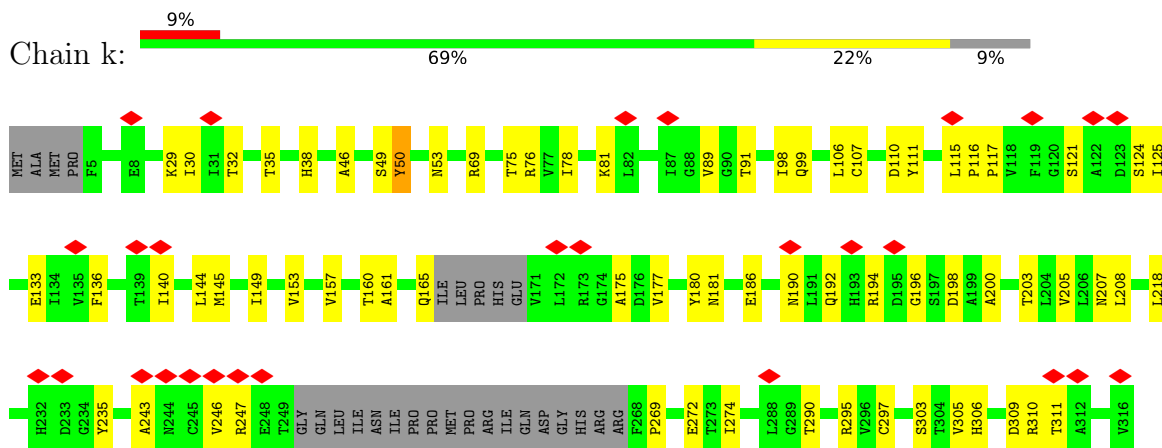
- Molecule 4: Triplex capsid protein 2

- Molecule 4: Triplex capsid protein 2

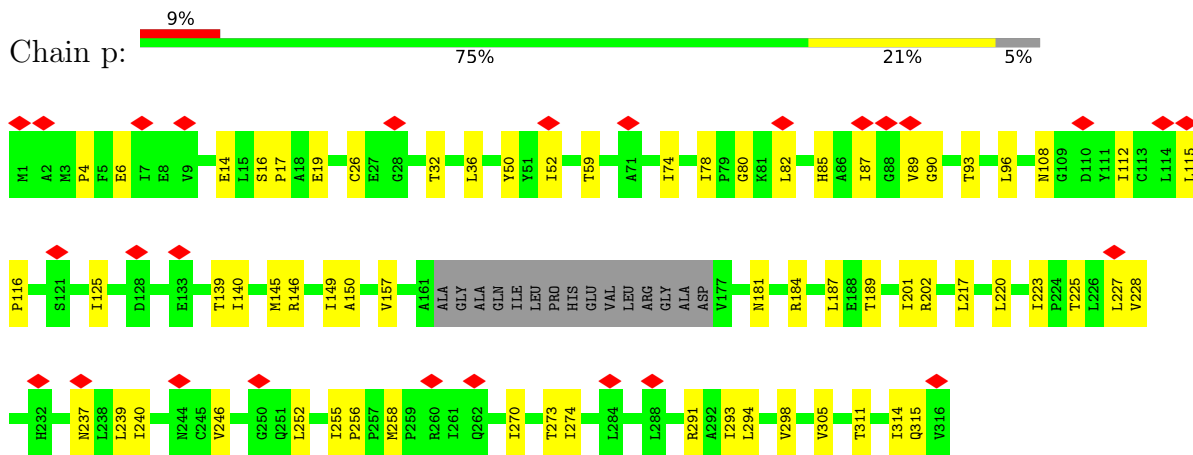




- Molecule 4: Triplex capsid protein 2

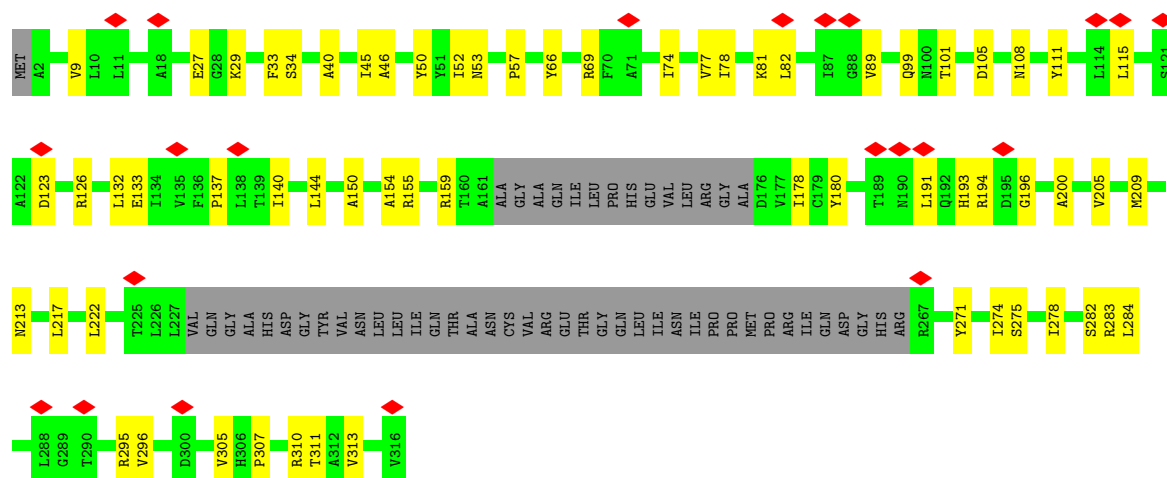


- Molecule 4: Triplex capsid protein 2

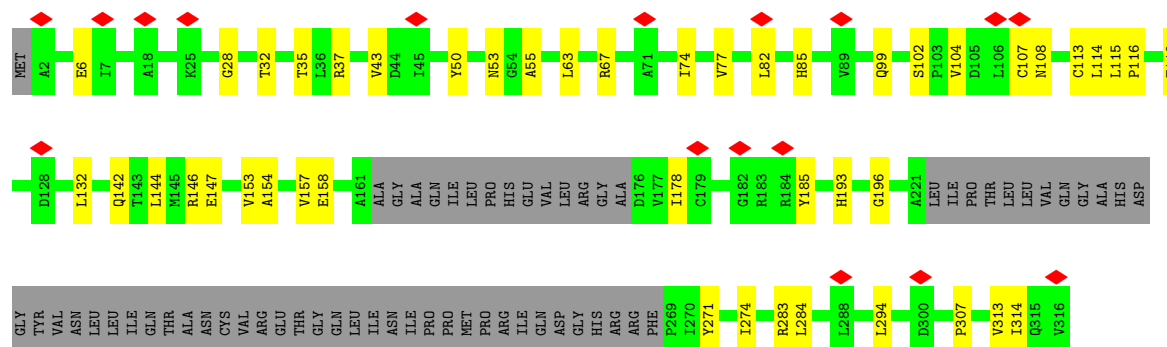


- Molecule 4: Triplex capsid protein 2

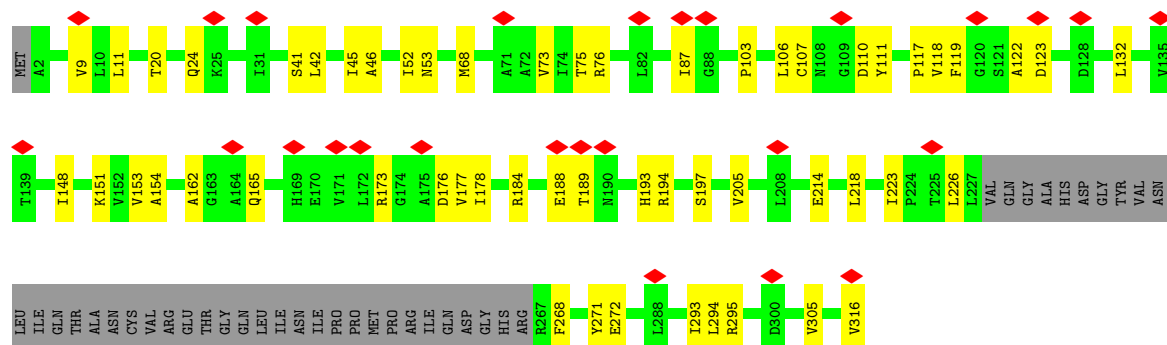




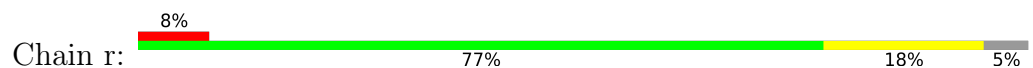
• Molecule 4: Triplex capsid protein 2

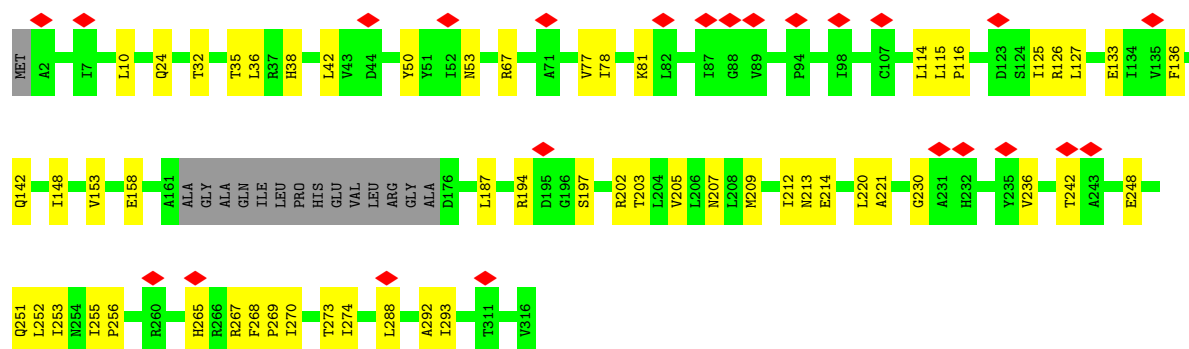


• Molecule 4: Triplex capsid protein 2

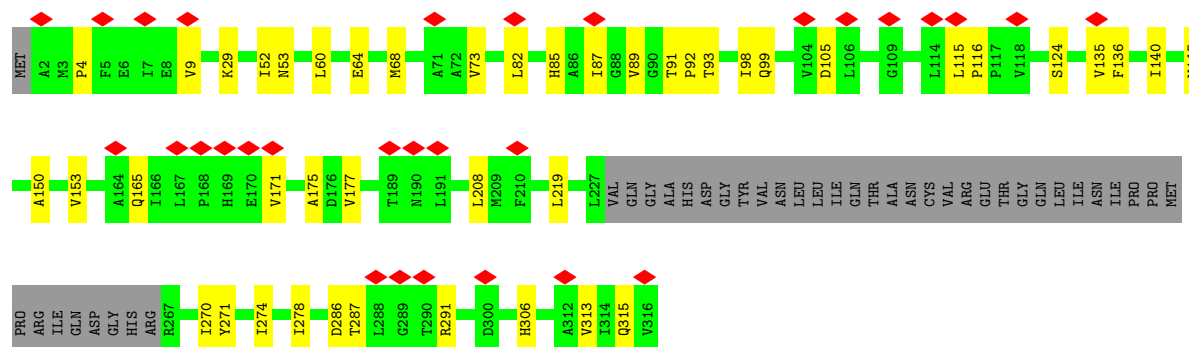


• Molecule 4: Triplex capsid protein 2

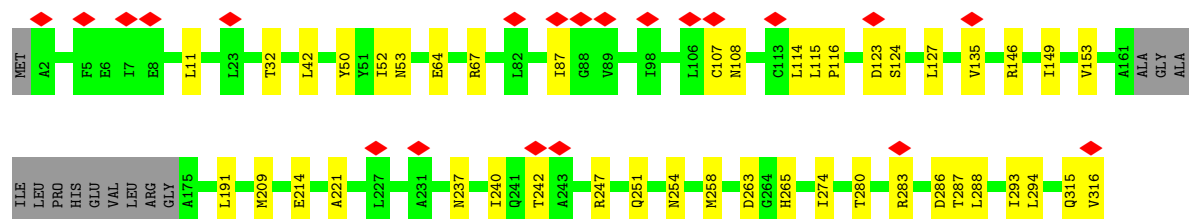
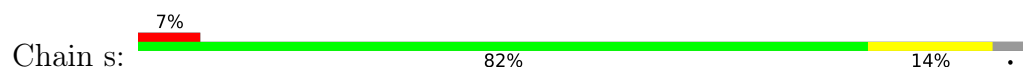




• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	22983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	22.144	Depositor
Minimum map value	-13.588	Depositor
Average map value	-0.009	Depositor
Map value standard deviation	1.978	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	1672.9601, 1672.9601, 1672.9601	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.307, 1.307, 1.307	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	0.26	0/10846	0.42	0/14767
1	B	0.20	0/10854	0.43	2/14778 (0.0%)
1	C	0.21	0/10846	0.43	0/14767
1	E	0.21	0/10834	0.43	1/14748 (0.0%)
1	F	0.20	0/10846	0.50	4/14767 (0.0%)
1	G	0.21	0/10377	0.50	2/14130 (0.0%)
1	M	0.26	0/10835	0.42	0/14752
1	N	0.24	0/10835	0.41	2/14752 (0.0%)
1	O	0.25	0/10854	0.41	0/14778
1	P	0.25	0/10854	0.42	0/14778
1	Q	0.27	0/10846	0.46	5/14767 (0.0%)
1	R	0.23	0/10835	0.43	0/14752
1	S	0.25	0/10854	0.41	0/14778
1	T	0.27	1/10846 (0.0%)	0.44	5/14767 (0.0%)
1	U	0.19	0/10675	0.46	0/14536
1	z	0.22	0/4800	0.57	2/6517 (0.0%)
2	D	0.19	0/782	0.50	0/1069
2	H	0.20	0/771	0.51	0/1055
2	I	0.21	0/782	0.51	0/1069
2	J	0.19	0/782	0.52	0/1069
2	K	0.23	0/782	0.54	0/1069
2	L	0.22	0/782	0.53	0/1069
2	V	0.18	0/782	0.47	1/1069 (0.1%)
2	W	0.22	0/782	0.46	0/1069
2	X	0.19	0/782	0.45	0/1069
2	Y	0.17	0/782	0.44	0/1069
2	Z	0.19	0/782	0.53	0/1069
2	a	0.19	0/782	0.46	0/1069
2	b	0.21	0/771	0.44	0/1055
2	c	0.18	0/782	0.46	0/1069
2	d	0.23	0/782	0.54	0/1069
3	e	0.18	0/2240	0.44	0/3034
3	f	0.22	0/2829	0.43	1/3843 (0.0%)
3	g	0.20	0/2470	0.42	0/3350

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	h	0.22	0/2746	0.40	0/3726
3	i	0.24	0/2851	0.40	0/3873
4	j	0.18	0/1868	0.46	0/2542
4	k	0.22	0/2236	0.39	0/3046
4	l	0.20	0/2041	0.41	0/2780
4	m	0.23	0/2144	0.42	0/2922
4	n	0.25	0/2144	0.44	1/2922 (0.0%)
4	o	0.19	0/2003	0.50	1/2727 (0.0%)
4	p	0.21	0/2350	0.39	0/3202
4	q	0.18	0/1971	0.36	0/2683
4	r	0.20	0/2350	0.40	0/3203
4	s	0.23	0/2355	0.39	0/3210
All	All	0.23	1/213143 (0.0%)	0.44	27/290204 (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	A	0	1
1	C	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	M	0	1
1	N	0	1
1	Q	0	1
1	S	0	2
1	T	0	2
4	k	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	1190	PRO	N-CD	12.25	1.65	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	1367	ALA	N-CA-C	8.36	122.91	111.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	1190	PRO	N-CA-CB	7.46	110.28	103.34
1	T	1189	ARG	N-CA-C	7.33	120.04	109.48
1	Q	1366	HIS	N-CA-C	7.28	119.93	108.79
1	T	1190	PRO	CA-N-CD	-6.75	102.55	112.00

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1394	LEU	Mainchain
1	M	1366	HIS	Peptide
1	N	1366	HIS	Peptide
1	Q	1394	LEU	Mainchain
1	S	1366	HIS	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	10592	0	10438	153	0
1	B	10600	0	10449	277	0
1	C	10592	0	10438	243	0
1	E	10582	0	10431	284	0
1	F	10592	0	10438	393	0
1	G	10133	0	9988	474	0
1	M	10582	0	10429	166	0
1	N	10582	0	10429	187	0
1	O	10600	0	10449	170	0
1	P	10600	0	10449	179	0
1	Q	10592	0	10438	169	0
1	R	10582	0	10429	212	0
1	S	10600	0	10449	184	0
1	T	10592	0	10438	202	0
1	U	10422	0	10256	382	0
1	z	4709	0	4688	134	0
2	D	765	0	777	26	0
2	H	754	0	764	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	765	0	777	27	0
2	J	765	0	777	29	0
2	K	765	0	777	33	0
2	L	765	0	777	30	0
2	V	765	0	777	32	0
2	W	765	0	777	17	0
2	X	765	0	777	24	0
2	Y	765	0	777	18	0
2	Z	765	0	777	19	0
2	a	765	0	777	22	0
2	b	754	0	764	28	0
2	c	765	0	777	21	0
2	d	765	0	777	38	0
3	e	2194	0	2172	47	0
3	f	2768	0	2721	58	0
3	g	2419	0	2380	60	0
3	h	2688	0	2639	62	0
3	i	2789	0	2736	48	0
4	j	1837	0	1909	67	0
4	k	2199	0	2259	47	0
4	l	2005	0	2069	44	0
4	m	2105	0	2174	36	0
4	n	2105	0	2174	26	0
4	o	1969	0	2031	73	0
4	p	2307	0	2379	47	0
4	q	1937	0	1990	33	0
4	r	2307	0	2371	44	0
4	s	2312	0	2376	31	0
All	All	208346	0	206645	4508	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 11.

The worst 5 of 4508 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)
1:G:510:GLU:CD	1:G:774:ARG:HH22	1.59	1.09
1:U:715:ARG:NH1	1:B:637:ARG:HH12	1.65	0.94
1:U:715:ARG:HH12	1:B:637:ARG:HH12	1.16	0.93
1:z:159:TYR:HE2	1:z:165:ILE:HD11	1.33	0.93
1:z:276:THR:HB	1:z:1087:ARG:HH22	1.36	0.91

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1350/1396 (97%)	1243 (92%)	106 (8%)	1 (0%)	48	83
1	B	1351/1396 (97%)	1236 (92%)	115 (8%)	0	100	100
1	C	1350/1396 (97%)	1226 (91%)	124 (9%)	0	100	100
1	E	1347/1396 (96%)	1214 (90%)	133 (10%)	0	100	100
1	F	1350/1396 (97%)	1189 (88%)	161 (12%)	0	100	100
1	G	1291/1396 (92%)	1118 (87%)	173 (13%)	0	100	100
1	M	1349/1396 (97%)	1237 (92%)	112 (8%)	0	100	100
1	N	1349/1396 (97%)	1239 (92%)	110 (8%)	0	100	100
1	O	1351/1396 (97%)	1255 (93%)	96 (7%)	0	100	100
1	P	1351/1396 (97%)	1254 (93%)	96 (7%)	1 (0%)	48	83
1	Q	1350/1396 (97%)	1232 (91%)	117 (9%)	1 (0%)	48	83
1	R	1349/1396 (97%)	1220 (90%)	128 (10%)	1 (0%)	48	83
1	S	1351/1396 (97%)	1236 (92%)	115 (8%)	0	100	100
1	T	1350/1396 (97%)	1216 (90%)	133 (10%)	1 (0%)	48	83
1	U	1327/1396 (95%)	1184 (89%)	141 (11%)	2 (0%)	43	77
1	z	595/1396 (43%)	521 (88%)	74 (12%)	0	100	100
2	D	98/235 (42%)	82 (84%)	16 (16%)	0	100	100
2	H	97/235 (41%)	82 (84%)	15 (16%)	0	100	100
2	I	98/235 (42%)	79 (81%)	19 (19%)	0	100	100
2	J	98/235 (42%)	82 (84%)	16 (16%)	0	100	100
2	K	98/235 (42%)	82 (84%)	16 (16%)	0	100	100
2	L	98/235 (42%)	82 (84%)	16 (16%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	98/235 (42%)	78 (80%)	20 (20%)	0	100	100
2	W	98/235 (42%)	84 (86%)	14 (14%)	0	100	100
2	X	98/235 (42%)	87 (89%)	11 (11%)	0	100	100
2	Y	98/235 (42%)	85 (87%)	13 (13%)	0	100	100
2	Z	98/235 (42%)	81 (83%)	17 (17%)	0	100	100
2	a	98/235 (42%)	79 (81%)	19 (19%)	0	100	100
2	b	97/235 (41%)	84 (87%)	13 (13%)	0	100	100
2	c	98/235 (42%)	81 (83%)	16 (16%)	1 (1%)	12	47
2	d	98/235 (42%)	81 (83%)	17 (17%)	0	100	100
3	e	267/483 (55%)	253 (95%)	14 (5%)	0	100	100
3	f	347/483 (72%)	319 (92%)	28 (8%)	0	100	100
3	g	303/483 (63%)	283 (93%)	20 (7%)	0	100	100
3	h	334/483 (69%)	310 (93%)	24 (7%)	0	100	100
3	i	349/483 (72%)	319 (91%)	30 (9%)	0	100	100
4	j	233/316 (74%)	220 (94%)	13 (6%)	0	100	100
4	k	283/316 (90%)	250 (88%)	33 (12%)	0	100	100
4	l	256/316 (81%)	228 (89%)	28 (11%)	0	100	100
4	m	272/316 (86%)	246 (90%)	26 (10%)	0	100	100
4	n	272/316 (86%)	247 (91%)	25 (9%)	0	100	100
4	o	250/316 (79%)	226 (90%)	24 (10%)	0	100	100
4	p	297/316 (94%)	289 (97%)	8 (3%)	0	100	100
4	q	248/316 (78%)	227 (92%)	21 (8%)	0	100	100
4	r	297/316 (94%)	278 (94%)	19 (6%)	0	100	100
4	s	298/316 (94%)	283 (95%)	15 (5%)	0	100	100
All	All	26535/31436 (84%)	24027 (90%)	2500 (9%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	48	PHE
1	U	49	ASP
2	c	17	THR
1	U	50	PHE
1	R	1302	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	1143/1182 (97%)	1143 (100%)	0	100	100
1	B	1144/1182 (97%)	1144 (100%)	0	100	100
1	C	1143/1182 (97%)	1142 (100%)	1 (0%)	88	88
1	E	1142/1182 (97%)	1142 (100%)	0	100	100
1	F	1143/1182 (97%)	1141 (100%)	2 (0%)	87	85
1	G	1092/1182 (92%)	1086 (100%)	6 (0%)	81	81
1	M	1142/1182 (97%)	1142 (100%)	0	100	100
1	N	1142/1182 (97%)	1141 (100%)	1 (0%)	88	88
1	O	1144/1182 (97%)	1144 (100%)	0	100	100
1	P	1144/1182 (97%)	1143 (100%)	1 (0%)	88	88
1	Q	1143/1182 (97%)	1142 (100%)	1 (0%)	88	88
1	R	1142/1182 (97%)	1141 (100%)	1 (0%)	88	88
1	S	1144/1182 (97%)	1144 (100%)	0	100	100
1	T	1143/1182 (97%)	1143 (100%)	0	100	100
1	U	1125/1182 (95%)	1125 (100%)	0	100	100
1	z	511/1182 (43%)	510 (100%)	1 (0%)	87	85
2	D	79/189 (42%)	79 (100%)	0	100	100
2	H	78/189 (41%)	78 (100%)	0	100	100
2	I	79/189 (42%)	79 (100%)	0	100	100
2	J	79/189 (42%)	79 (100%)	0	100	100
2	K	79/189 (42%)	79 (100%)	0	100	100
2	L	79/189 (42%)	79 (100%)	0	100	100
2	V	79/189 (42%)	79 (100%)	0	100	100
2	W	79/189 (42%)	79 (100%)	0	100	100
2	X	79/189 (42%)	79 (100%)	0	100	100
2	Y	79/189 (42%)	79 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Z	79/189 (42%)	79 (100%)	0	100	100
2	a	79/189 (42%)	79 (100%)	0	100	100
2	b	78/189 (41%)	78 (100%)	0	100	100
2	c	79/189 (42%)	79 (100%)	0	100	100
2	d	79/189 (42%)	78 (99%)	1 (1%)	61	72
3	e	235/410 (57%)	235 (100%)	0	100	100
3	f	294/410 (72%)	294 (100%)	0	100	100
3	g	256/410 (62%)	256 (100%)	0	100	100
3	h	285/410 (70%)	285 (100%)	0	100	100
3	i	296/410 (72%)	296 (100%)	0	100	100
4	j	205/267 (77%)	205 (100%)	0	100	100
4	k	243/267 (91%)	243 (100%)	0	100	100
4	l	224/267 (84%)	224 (100%)	0	100	100
4	m	233/267 (87%)	233 (100%)	0	100	100
4	n	233/267 (87%)	233 (100%)	0	100	100
4	o	220/267 (82%)	218 (99%)	2 (1%)	70	76
4	p	257/267 (96%)	257 (100%)	0	100	100
4	q	216/267 (81%)	216 (100%)	0	100	100
4	r	257/267 (96%)	257 (100%)	0	100	100
4	s	257/267 (96%)	257 (100%)	0	100	100
All	All	22481/26467 (85%)	22464 (100%)	17 (0%)	87	88

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	o	9	VAL
1	z	392	VAL
1	F	1388	LEU
1	G	510	GLU
1	G	928	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 492 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	1366	HIS
3	g	273	ASN
1	B	1306	ASN
4	p	181	ASN
3	i	414	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

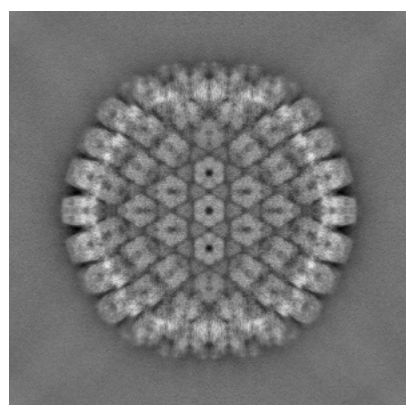
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0880. These allow visual inspection of the internal detail of the map and identification of artifacts.

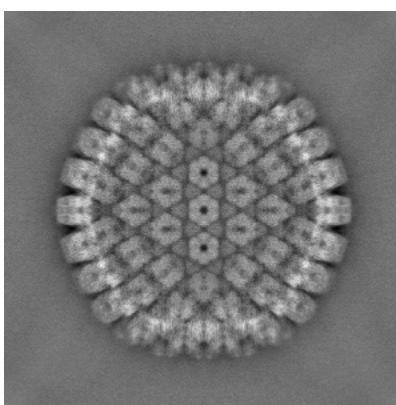
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

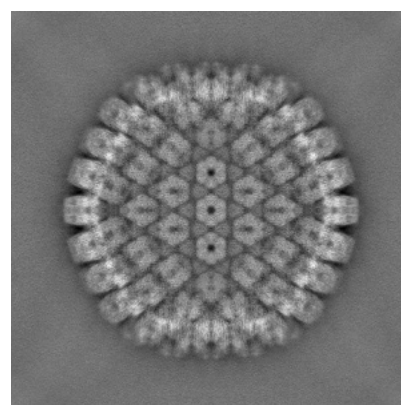
6.1.1 Primary map



X



Y

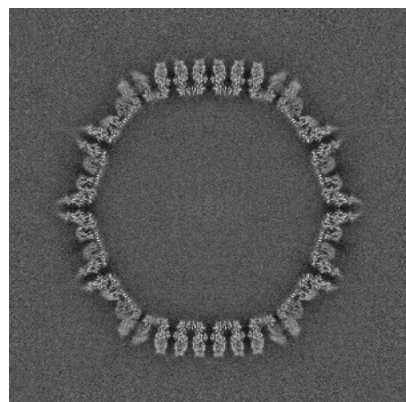


Z

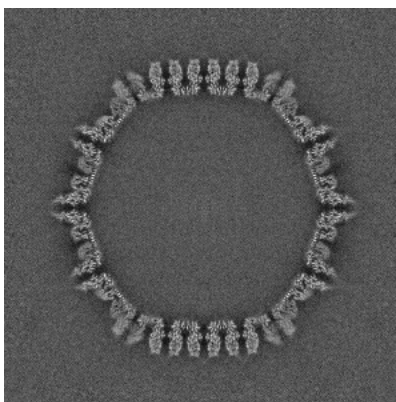
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

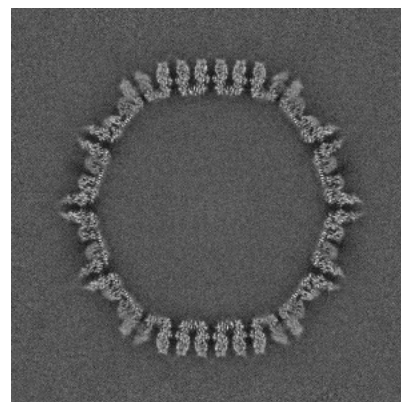
6.2.1 Primary map



X Index: 640



Y Index: 640

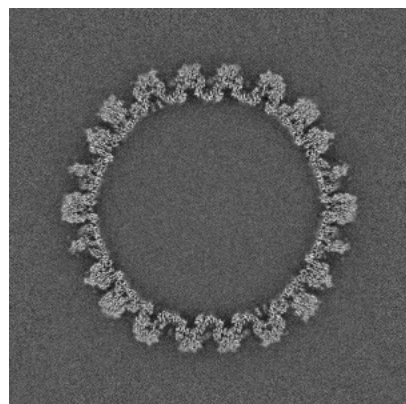


Z Index: 640

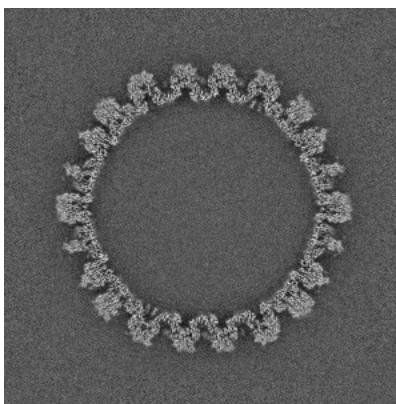
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

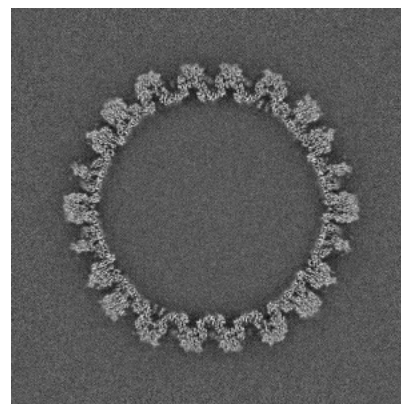
6.3.1 Primary map



X Index: 537



Y Index: 743

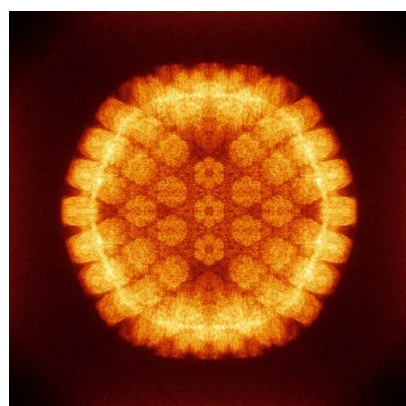


Z Index: 742

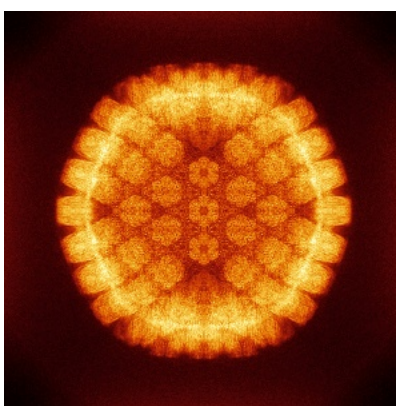
The images above show the largest variance slices of the map in three orthogonal directions.

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

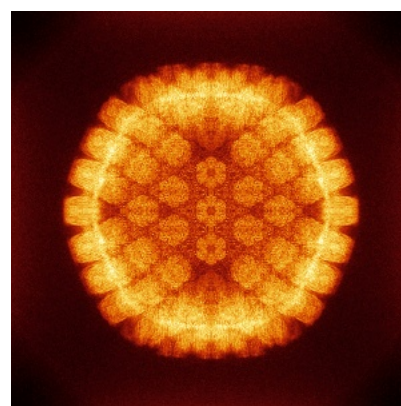
6.4.1 Primary map



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

This section was not generated.

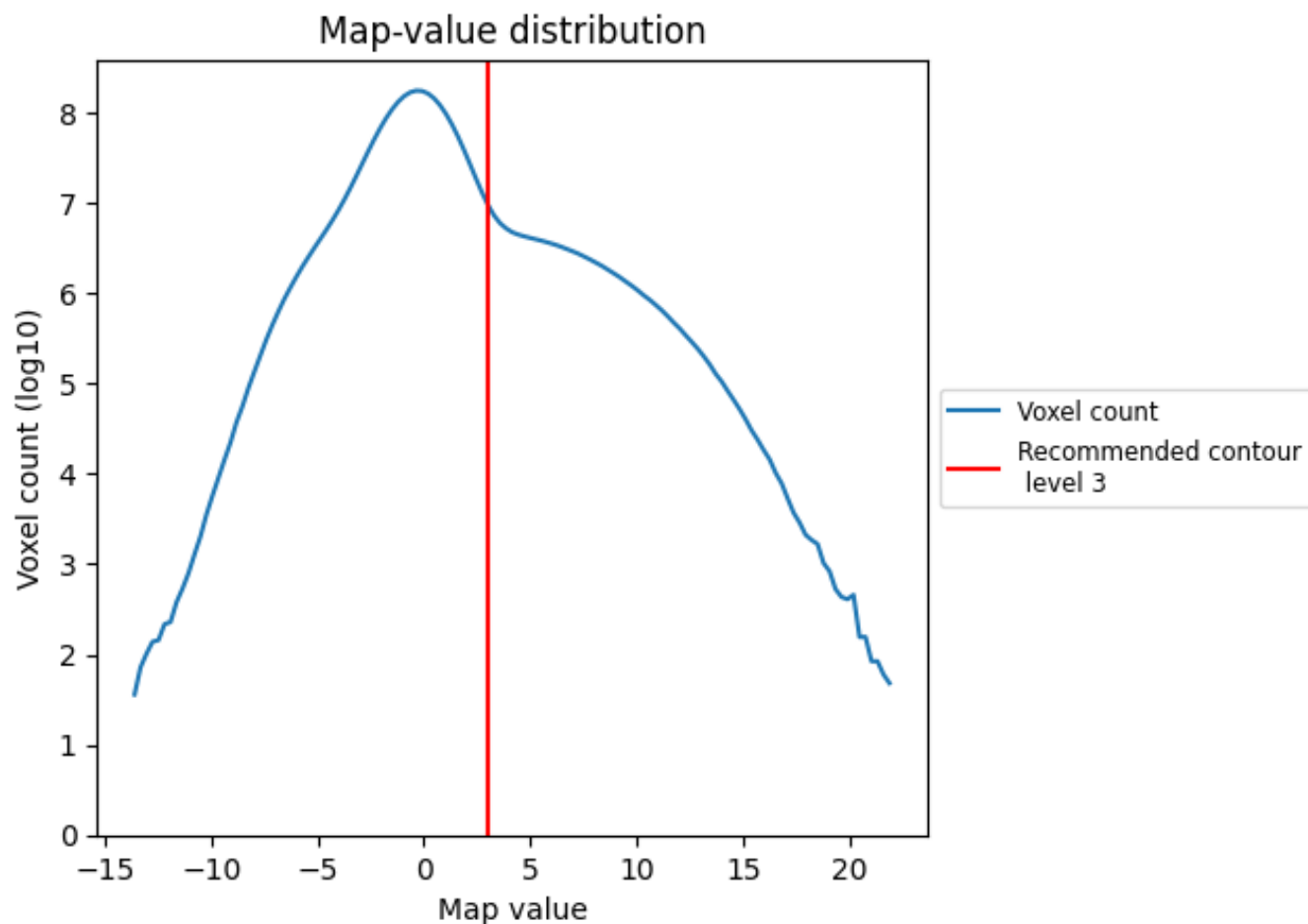
6.6 Mask visualisation

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

7 Map analysis [i](#)

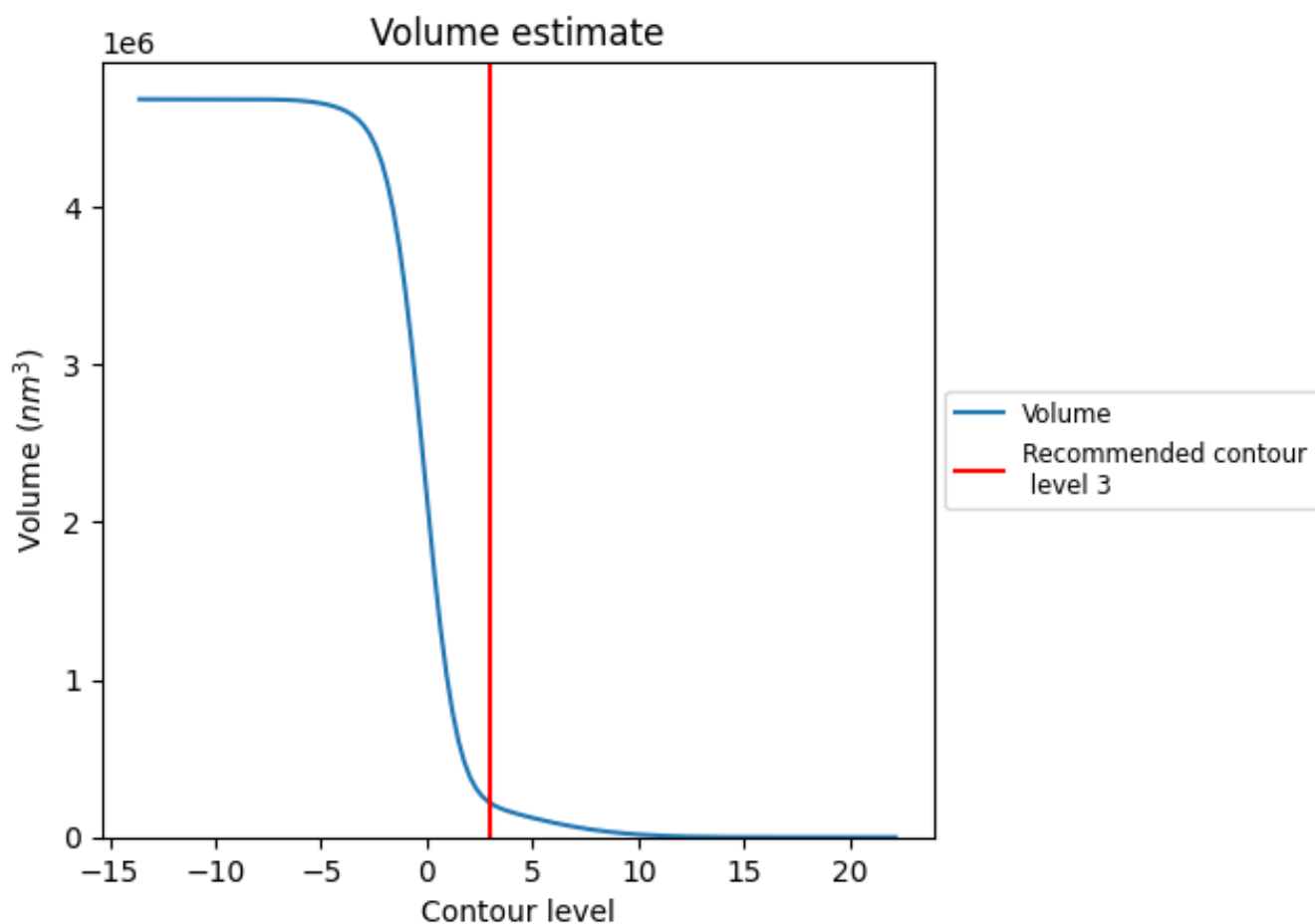
This section contains the results of statistical analysis of the map.

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.

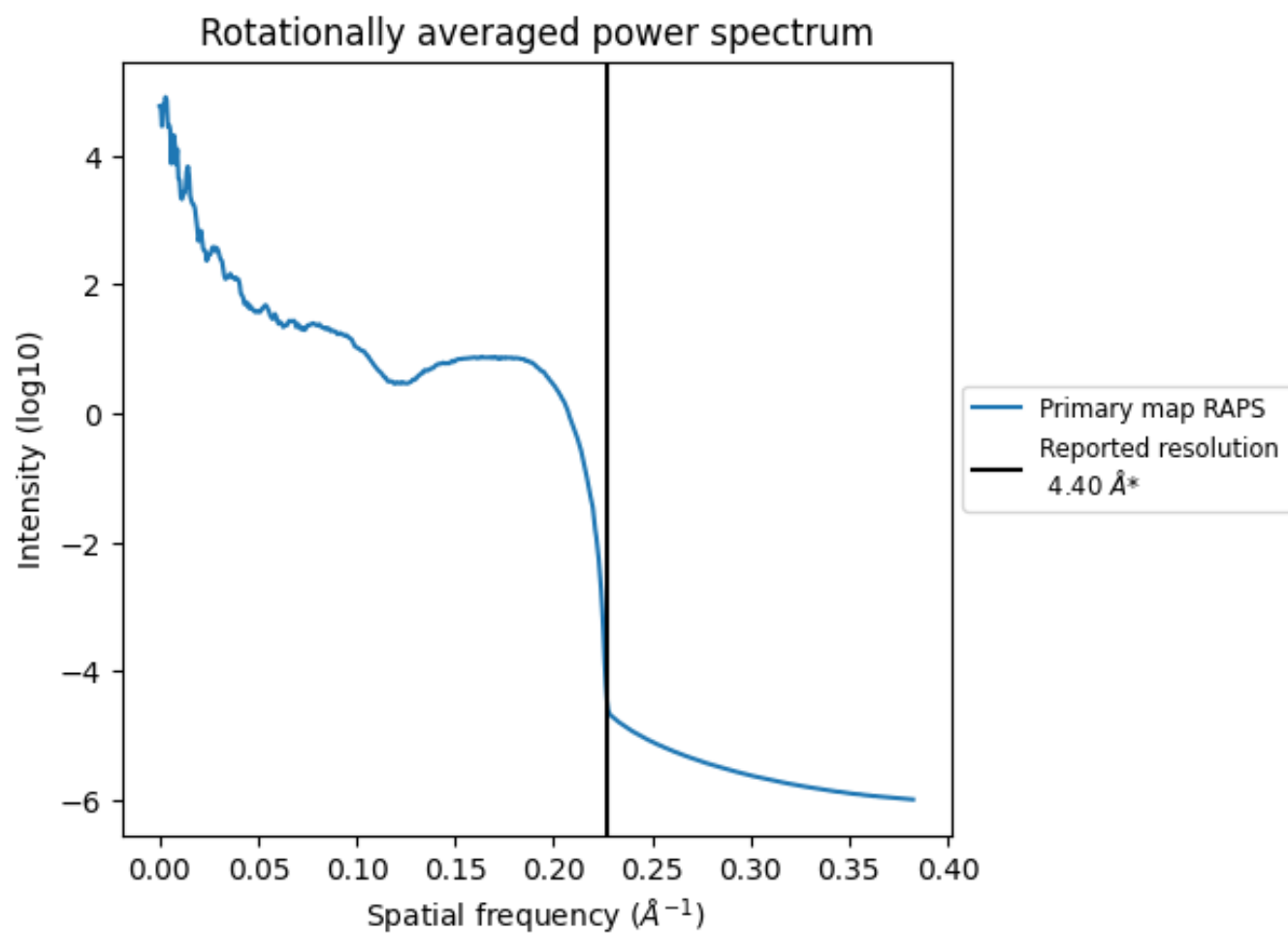
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 217083 nm³; this corresponds to an approximate mass of 196097 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 0.227 Å⁻¹

8 Fourier-Shell correlation

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

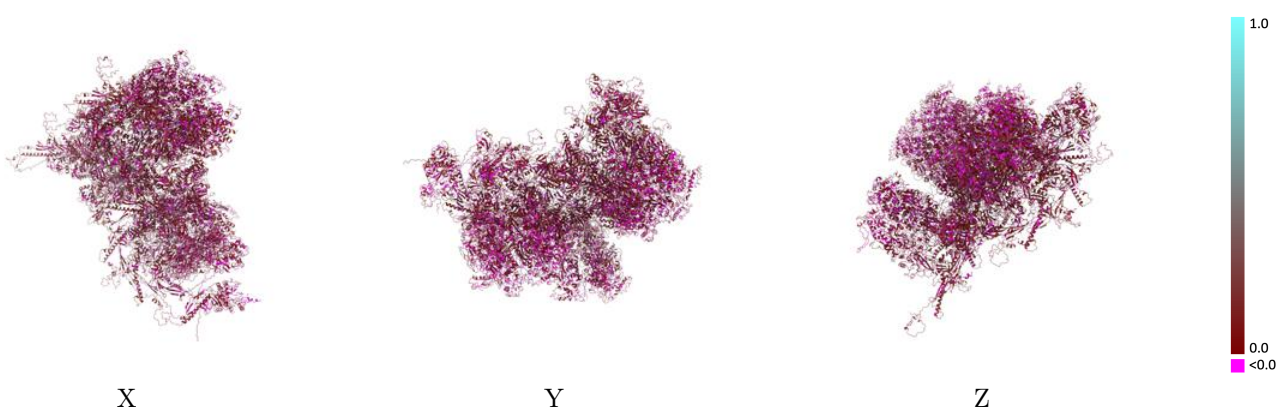
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0880 and PDB model 6LGL. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

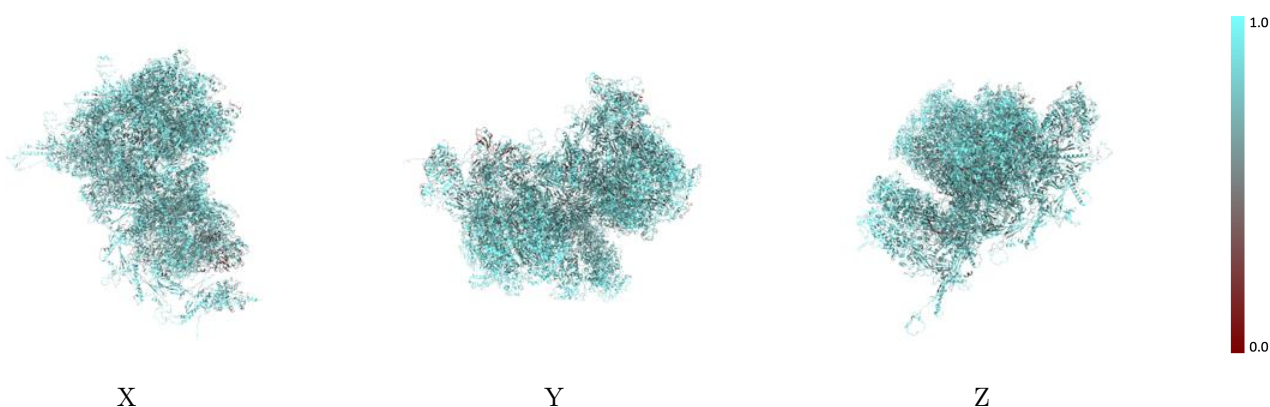
This section was not generated.

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



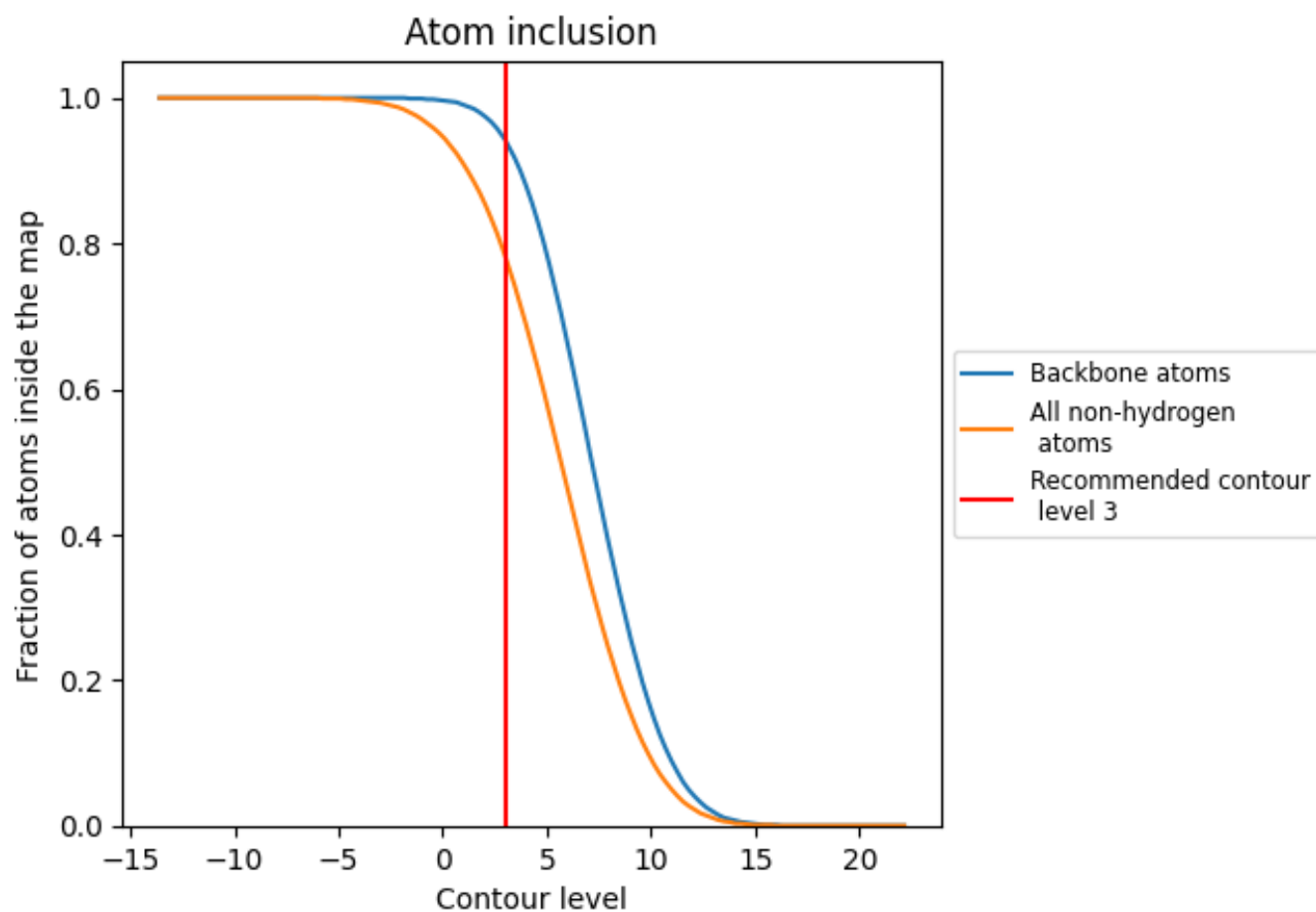
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 78% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7820	 0.1140
A	 0.7860	 0.1250
B	 0.8090	 0.1040
C	 0.7990	 0.1140
D	 0.7720	 0.0790
E	 0.7850	 0.1150
F	 0.7950	 0.1040
G	 0.8010	 0.0950
H	 0.8990	 0.0650
I	 0.8930	 0.0840
J	 0.8740	 0.0690
K	 0.8780	 0.0920
L	 0.8580	 0.0630
M	 0.7880	 0.1210
N	 0.8060	 0.1210
O	 0.7980	 0.1170
P	 0.8040	 0.1140
Q	 0.7940	 0.1200
R	 0.7910	 0.1220
S	 0.7980	 0.1220
T	 0.7950	 0.1230
U	 0.7990	 0.1000
V	 0.7230	 0.0870
W	 0.7460	 0.0560
X	 0.7420	 0.0480
Y	 0.7630	 0.0730
Z	 0.7690	 0.0600
a	 0.8570	 0.0910
b	 0.8650	 0.0990
c	 0.8610	 0.0560
d	 0.9090	 0.0780
e	 0.5730	 0.1210
f	 0.7440	 0.1350
g	 0.7840	 0.1210
h	 0.7460	 0.1330



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7320	 0.1340
j	 0.5380	 0.1010
k	 0.7170	 0.1360
l	 0.7550	 0.1290
m	 0.7270	 0.1400
n	 0.7270	 0.1370
o	 0.5270	 0.1070
p	 0.7370	 0.1420
q	 0.7640	 0.1310
r	 0.7270	 0.1320
s	 0.7360	 0.1410
z	 0.7260	 0.0980