



## wwPDB EM Validation Summary Report ⓘ

Oct 1, 2024 – 02:46 PM JST

PDB ID : 5ZAP  
EMDB ID : EMD-6907  
Title : Atomic structure of the herpes simplex virus type 2 B-capsid  
Authors : Yuan, S.; Wang, J.L.; Zhu, D.J.; Wang, N.; Gao, Q.; Chen, W.Y.; Tang, H.;  
Wang, J.Z.; Zhang, X.Z.; Liu, H.R.; Rao, Z.H.; Wang, X.X.  
Deposited on : 2018-02-08  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

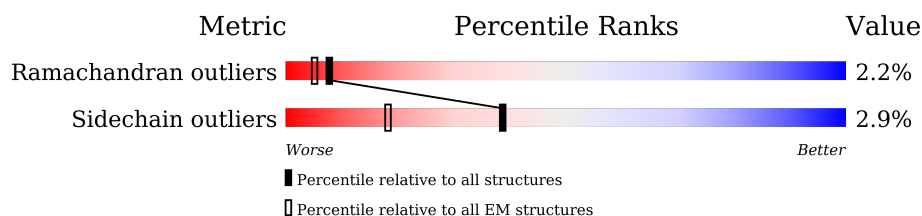
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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  $\geq 3$ , 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	1374	<div> <div>19%</div> <div>95%</div> </div>
1	B	1374	<div> <div>16%</div> <div>93%</div> </div>
1	C	1374	<div> <div>15%</div> <div>95%</div> </div>
1	D	1374	<div> <div>18%</div> <div>94%</div> <div>5%</div> </div>
1	E	1374	<div> <div>18%</div> <div>95%</div> </div>
1	F	1374	<div> <div>15%</div> <div>95%</div> </div>
1	G	1374	<div> <div>48%</div> <div>93%</div> <div>5%</div> </div>
1	H	1374	<div> <div>21%</div> <div>95%</div> </div>
1	I	1374	<div> <div>14%</div> <div>94%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	J	1374	
1	K	1374	
1	L	1374	
1	M	1374	
1	N	1374	
1	O	1374	
1	P	1374	
2	Q	318	
2	R	318	
2	T	318	
2	U	318	
2	W	318	
2	X	318	
2	Z	318	
2	a	318	
2	c	318	
2	d	318	
3	S	466	
3	V	466	
3	Y	466	
3	b	466	
3	e	466	
4	f	112	
4	g	112	
4	h	112	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	i	112	<div>88%</div> <div>71%21% . .</div>
4	j	112	<div>91%</div> <div>71%21% . .</div>
4	k	112	<div>89%</div> <div>69%24% . .</div>
4	l	112	<div>88%</div> <div>71%21% . .</div>
4	m	112	<div>94%</div> <div>71%22% . .</div>
4	n	112	<div>93%</div> <div>71%22% . .</div>
4	o	112	<div>92%</div> <div>70%21% . .</div>
4	p	112	<div>87%</div> <div>71%22% . .</div>
4	q	112	<div>88%</div> <div>71%22% . .</div>
4	r	112	<div>88%</div> <div>66%27% . .</div>
4	s	112	<div>90%</div> <div>72%21% . .</div>
4	t	112	<div>88%</div> <div>70%22% . .</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 205925 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	G	1365	Total 10104	C 6424	N 1819	O 1807	S 54	0	0
1	A	1365	Total 10160	C 6460	N 1837	O 1809	S 54	0	0
1	B	1350	Total 10105	C 6411	N 1825	O 1815	S 54	0	0
1	C	1362	Total 10220	C 6484	N 1852	O 1829	S 55	0	0
1	D	1362	Total 10229	C 6488	N 1849	O 1837	S 55	0	0
1	E	1362	Total 10233	C 6490	N 1853	O 1835	S 55	0	0
1	F	1362	Total 10239	C 6494	N 1857	O 1833	S 55	0	0
1	H	1362	Total 10245	C 6498	N 1851	O 1841	S 55	0	0
1	I	1361	Total 10239	C 6494	N 1850	O 1840	S 55	0	0
1	J	1362	Total 10204	C 6477	N 1842	O 1831	S 54	0	0
1	K	1362	Total 10253	C 6502	N 1857	O 1839	S 55	0	0
1	L	1362	Total 10242	C 6493	N 1851	O 1843	S 55	0	0
1	M	1365	Total 10275	C 6515	N 1859	O 1846	S 55	0	0
1	N	1362	Total 10254	C 6499	N 1857	O 1843	S 55	0	0
1	O	1362	Total 10251	C 6500	N 1859	O 1837	S 55	0	0
1	P	1362	Total 10256	C 6502	N 1855	O 1844	S 55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
2	R	307	Total	C	N	O	S	0	0
			2175	1405	392	370	8		
2	T	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
2	U	307	Total	C	N	O	S	0	0
			2179	1407	393	371	8		
2	W	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
2	X	308	Total	C	N	O	S	0	0
			2187	1411	394	374	8		
2	Z	299	Total	C	N	O	S	0	0
			2063	1334	366	356	7		
2	a	307	Total	C	N	O	S	0	0
			2169	1402	389	370	8		
2	c	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
2	d	308	Total	C	N	O	S	0	0
			2187	1411	394	374	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	329	Total	C	N	O	S	0	0
			2267	1437	411	402	17		
3	V	346	Total	C	N	O	S	0	0
			2365	1500	432	416	17		
3	Y	347	Total	C	N	O	S	0	0
			2386	1512	437	420	17		
3	b	343	Total	C	N	O	S	0	0
			2331	1478	421	416	16		
3	e	343	Total	C	N	O	S	0	0
			2364	1497	435	415	17		

- Molecule 4 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	g	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	h	107	Total	C	N	O	S	0	0
			628	387	119	120	2		

*Continued on next page...*

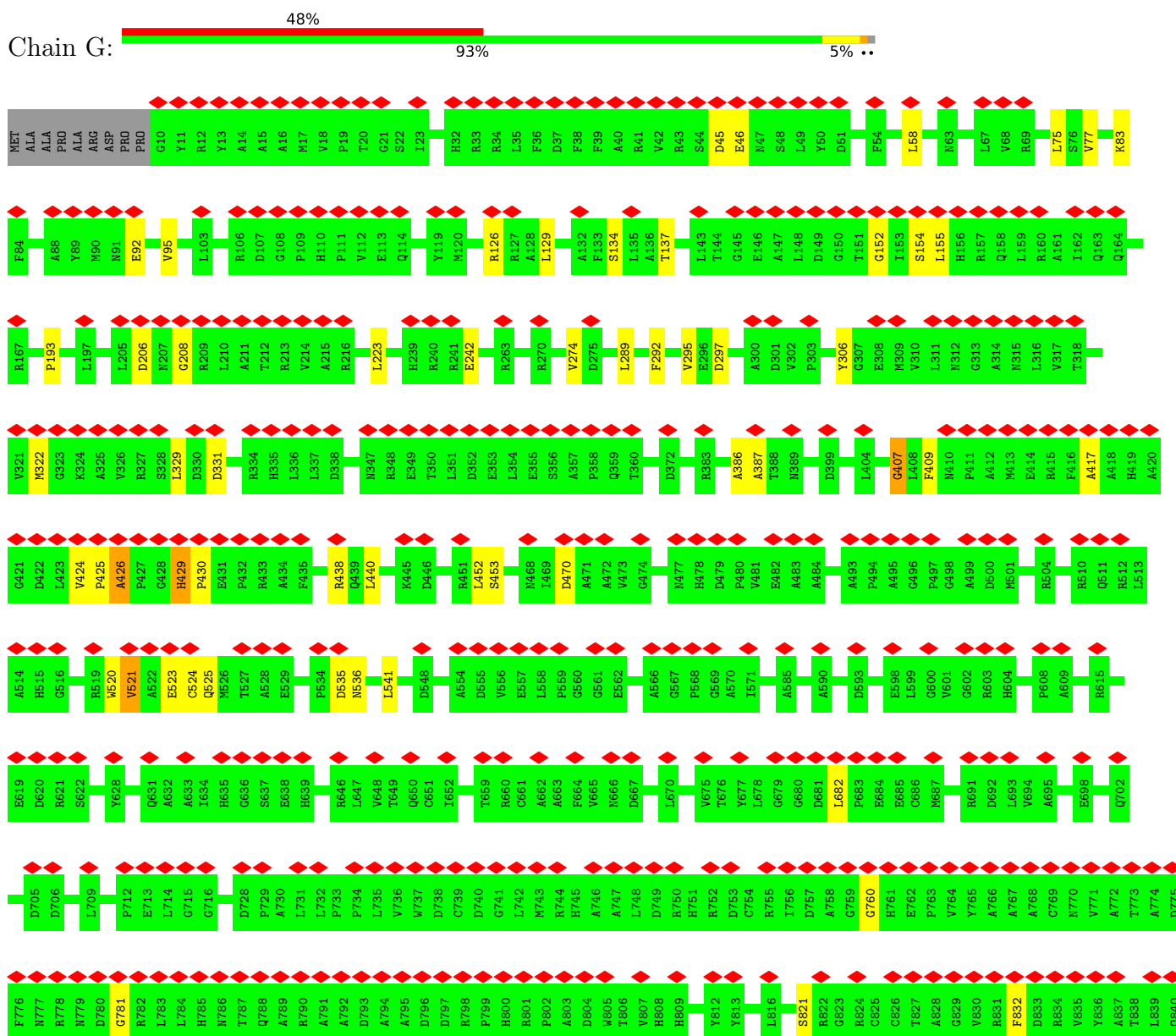
*Continued from previous page...*

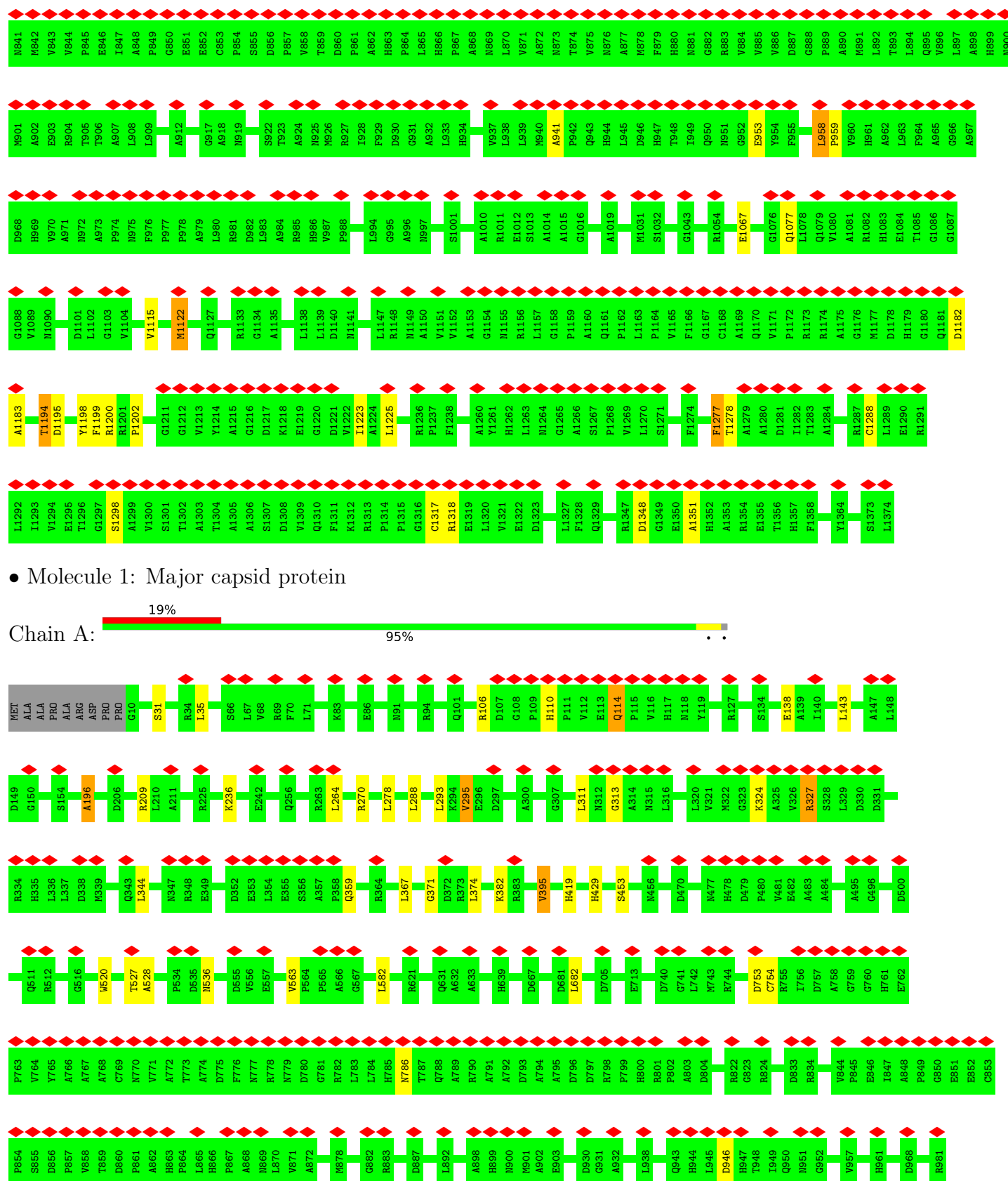
Mol	Chain	Residues	Atoms					AltConf	Trace
4	i	107	Total 628	C 387	N 119	O 120	S 2	0	0
4	j	107	Total 632	C 390	N 120	O 120	S 2	0	0
4	k	107	Total 628	C 387	N 119	O 120	S 2	0	0
4	l	107	Total 628	C 387	N 119	O 120	S 2	0	0
4	m	107	Total 628	C 387	N 119	O 120	S 2	0	0
4	n	107	Total 625	C 385	N 119	O 120	S 1	0	0
4	o	107	Total 628	C 387	N 119	O 120	S 2	0	0
4	p	107	Total 628	C 387	N 119	O 120	S 2	0	0
4	q	107	Total 628	C 387	N 119	O 120	S 2	0	0
4	r	107	Total 632	C 390	N 120	O 120	S 2	0	0
4	s	107	Total 634	C 390	N 122	O 120	S 2	0	0
4	t	107	Total 628	C 387	N 119	O 120	S 2	0	0

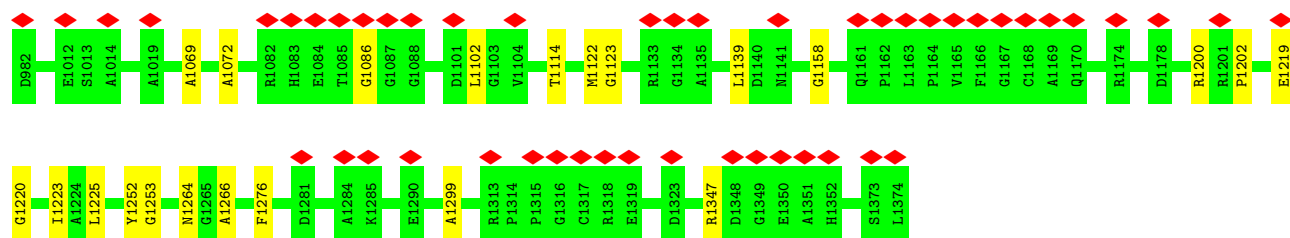
### 3 Residue-property plots [i](#)

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.

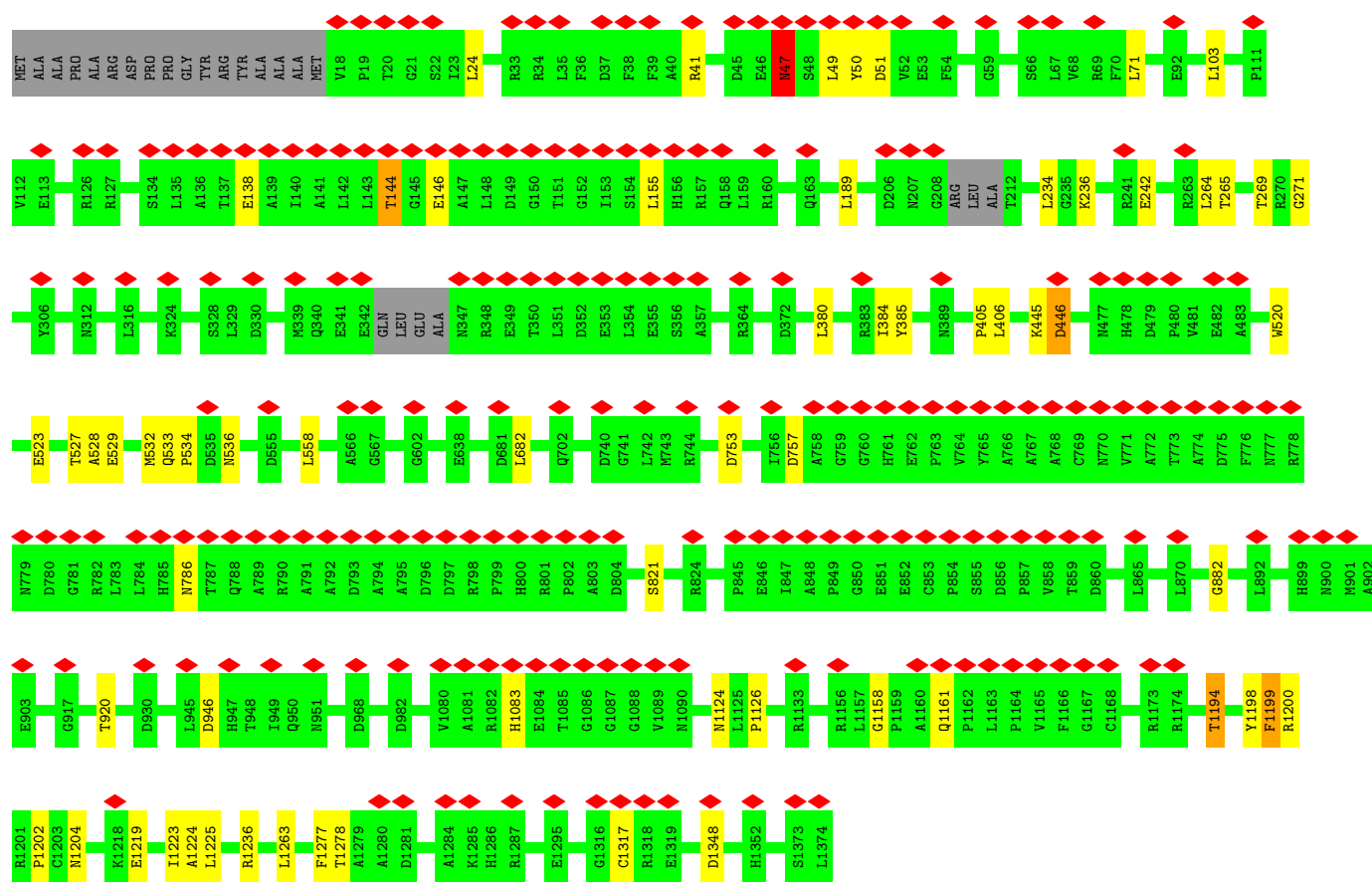
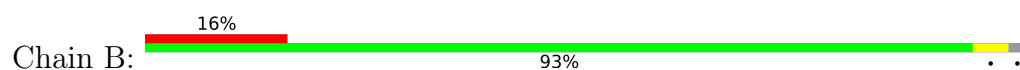
#### • Molecule 1: Major capsid protein



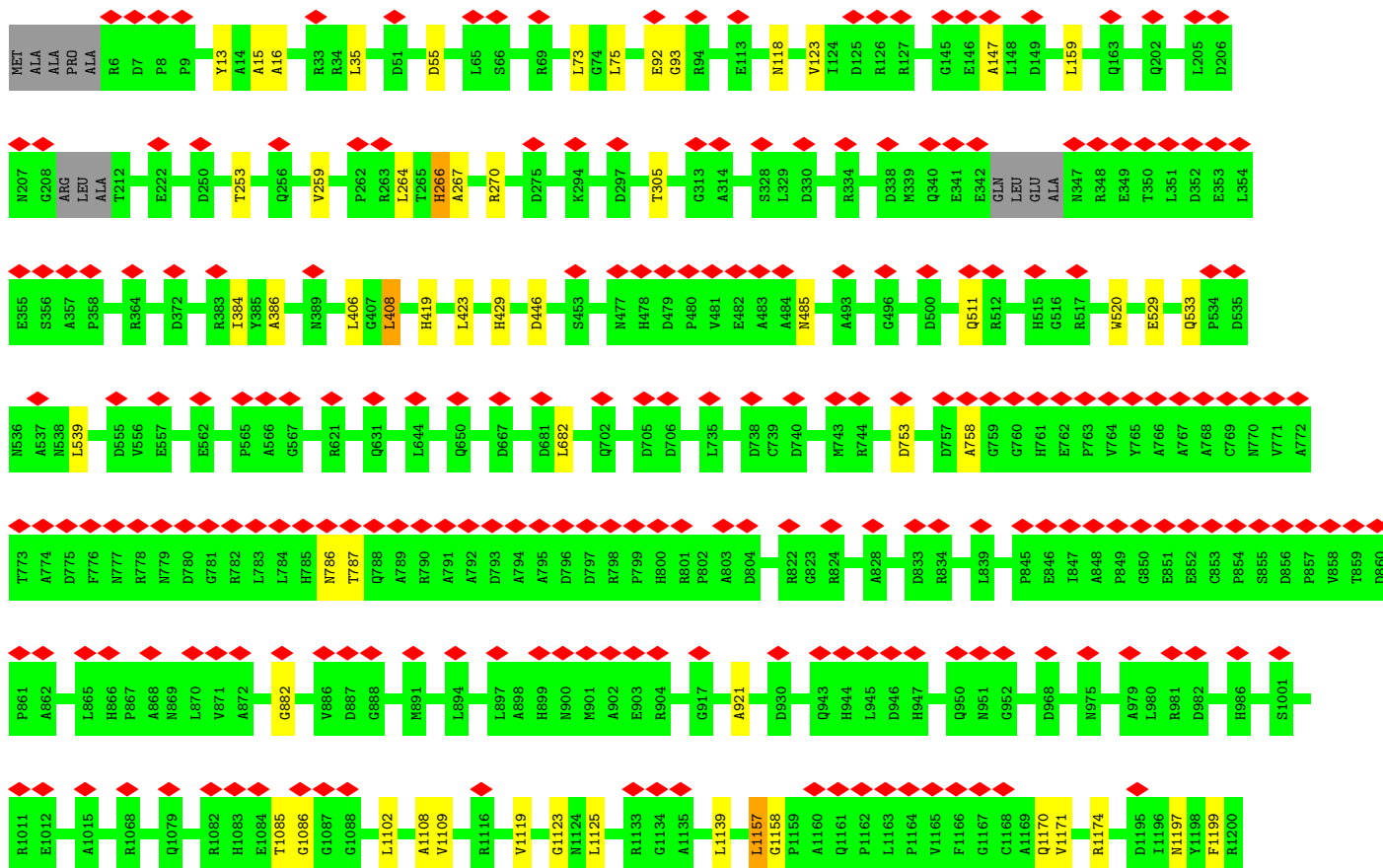
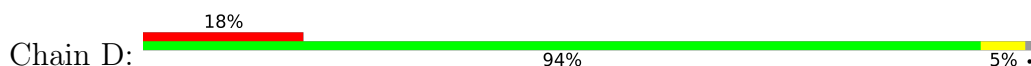


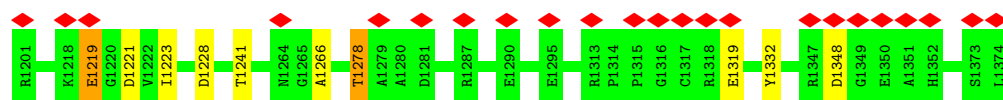


• Molecule 1: Major capsid protein

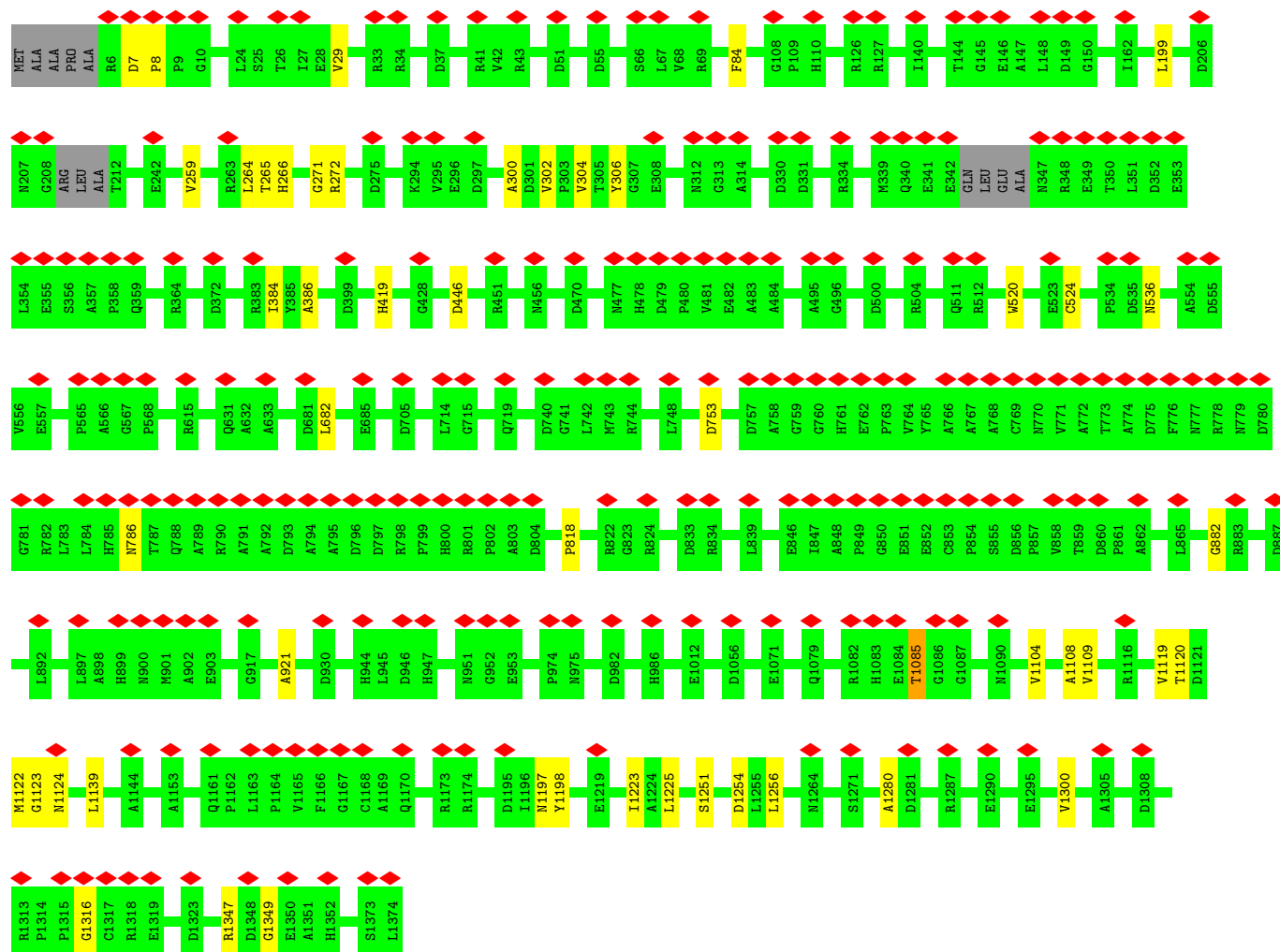


- Molecule 1: Major capsid protein

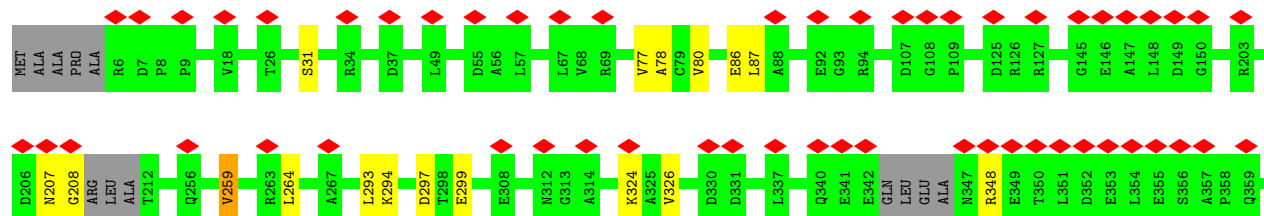


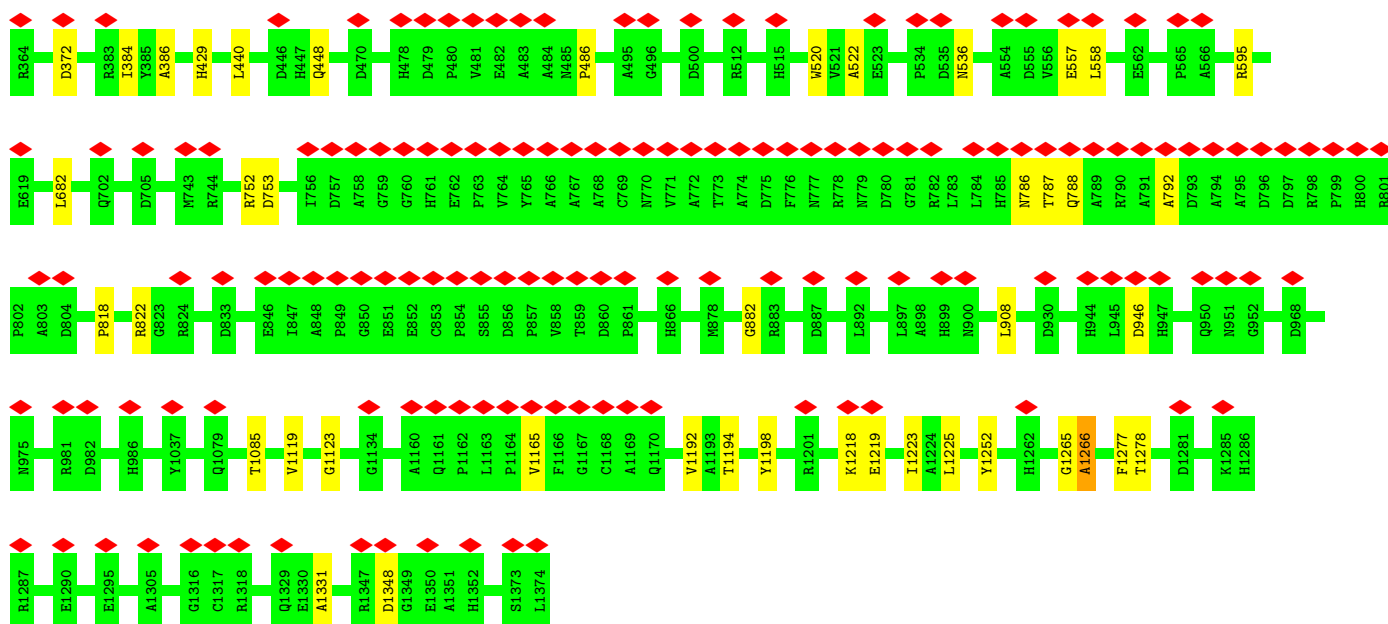


• Molecule 1: Major capsid protein

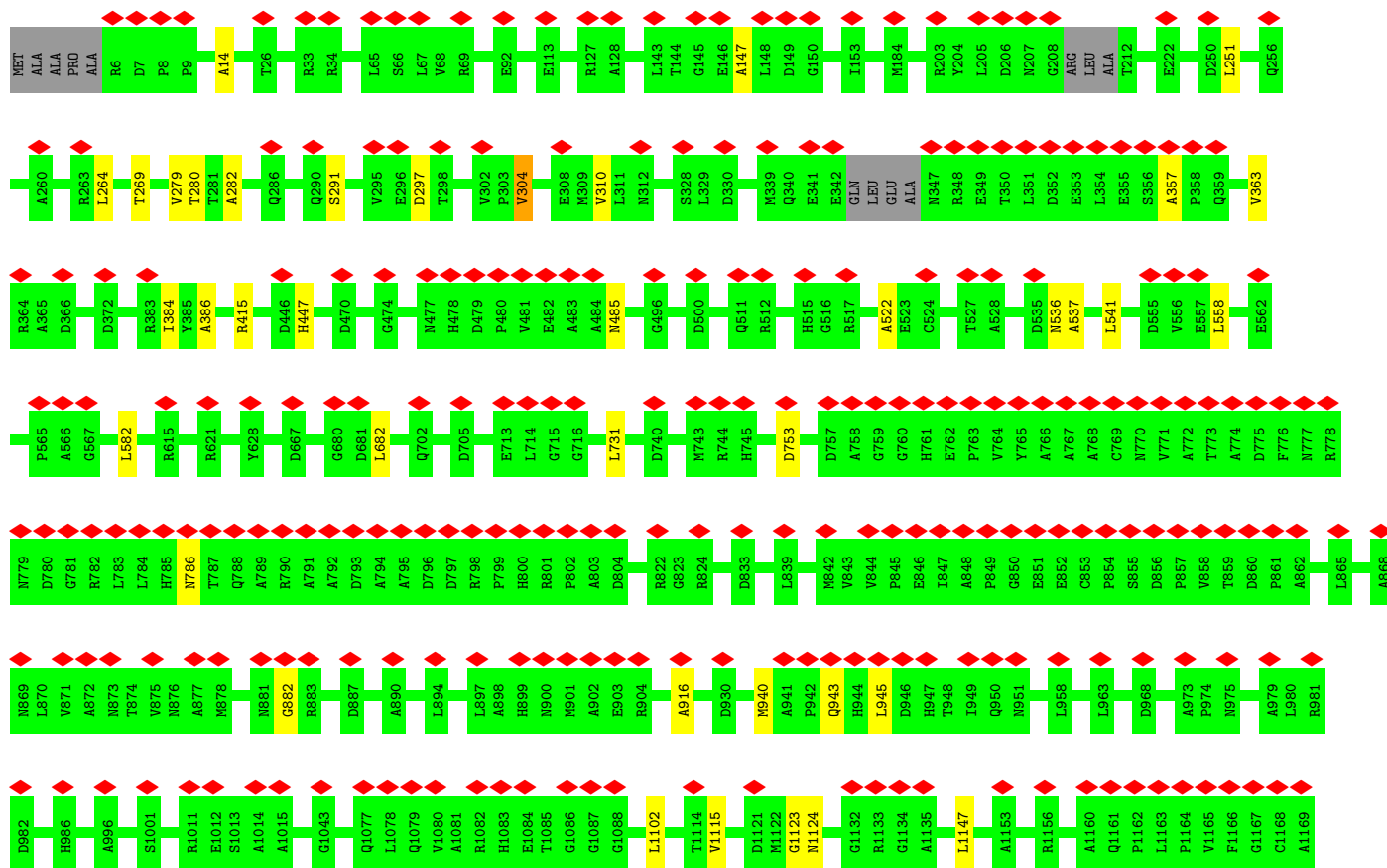


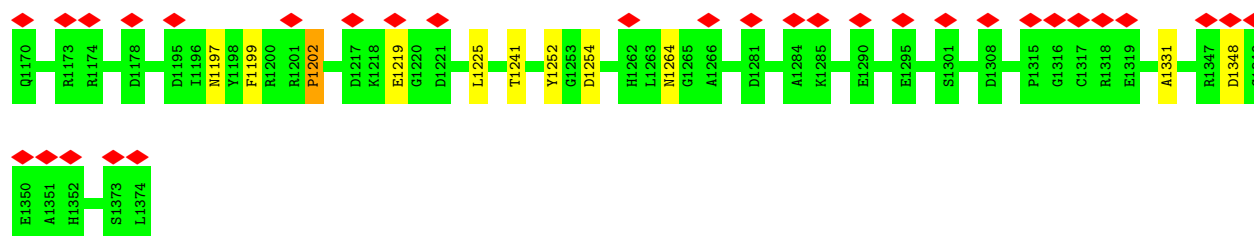
• Molecule 1: Major capsid protein



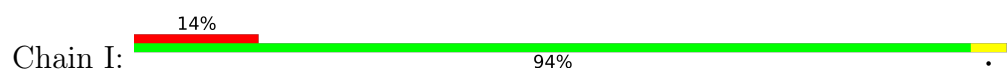


• Molecule 1: Major capsid protein

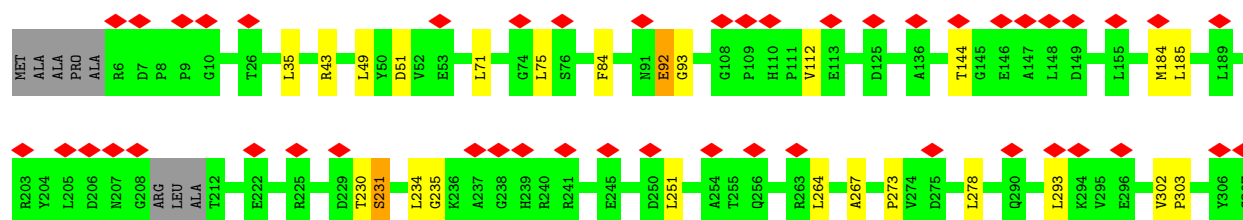


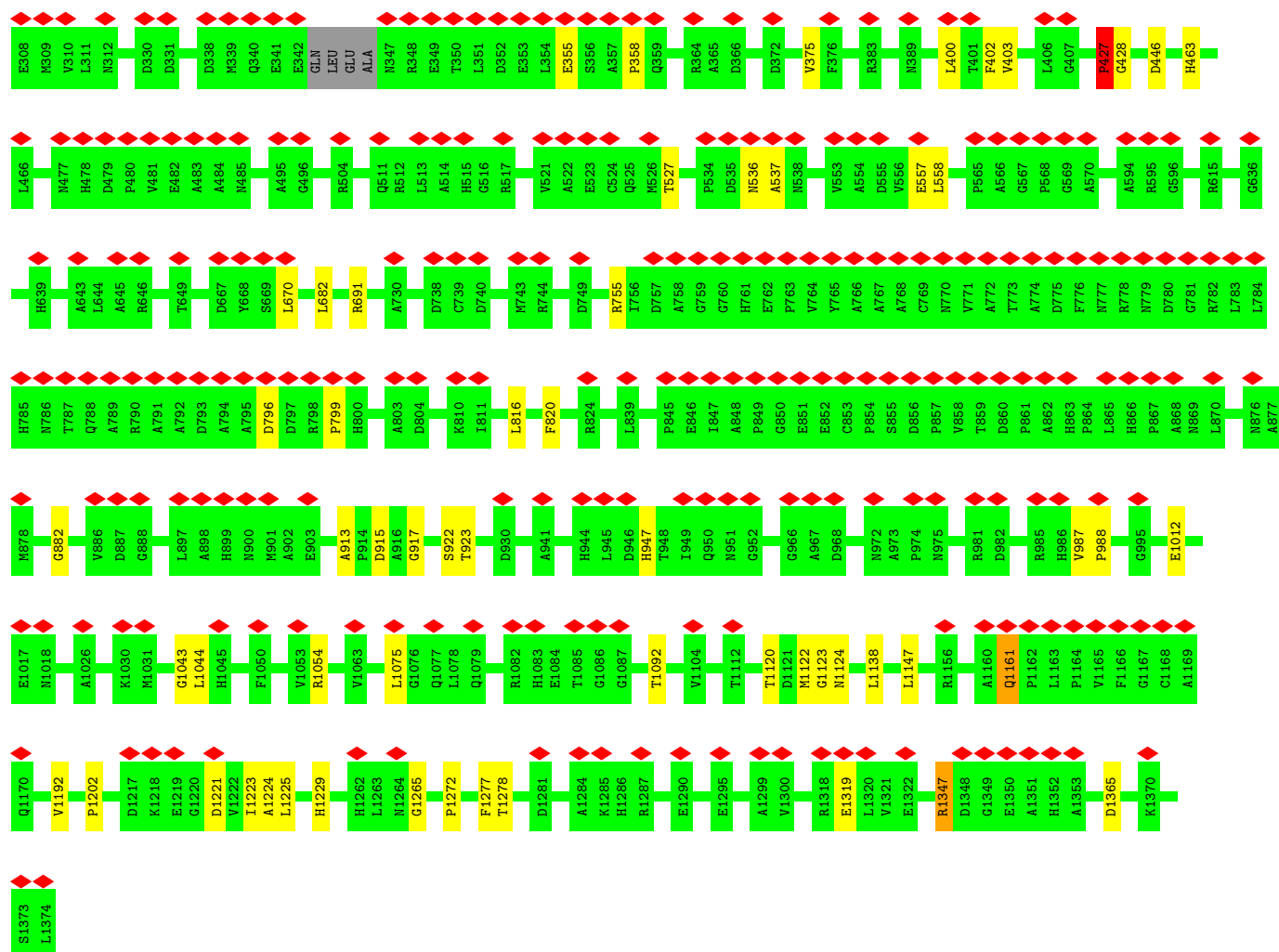


• Molecule 1: Major capsid protein



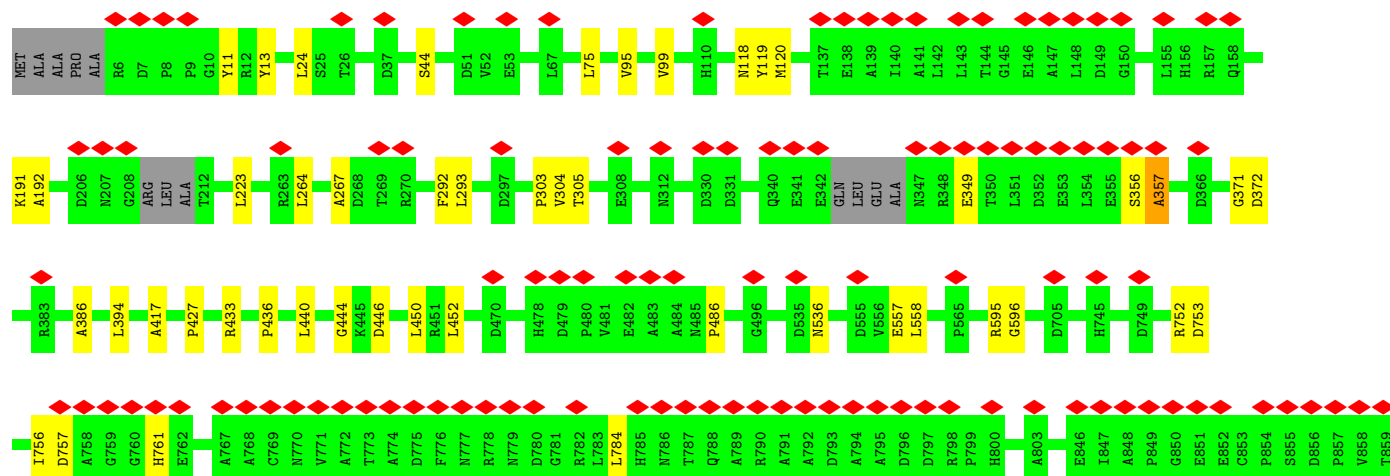
• Molecule 1: Major capsid protein

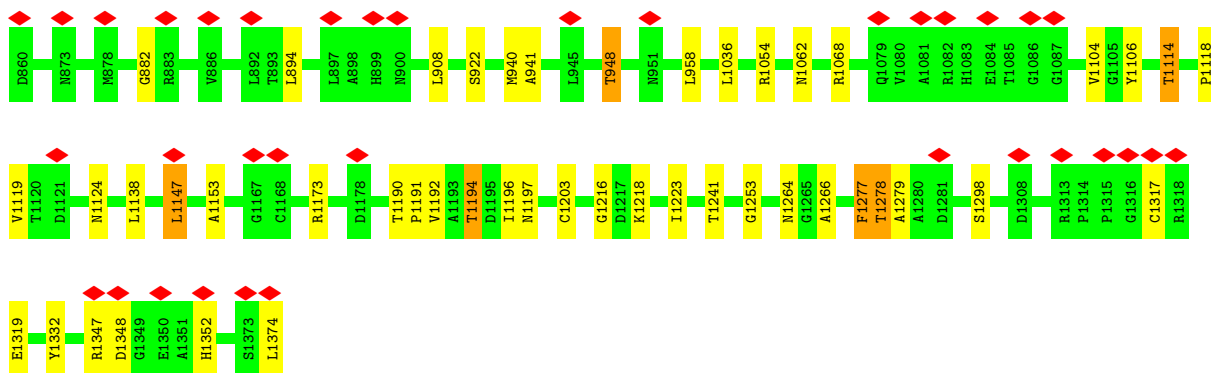




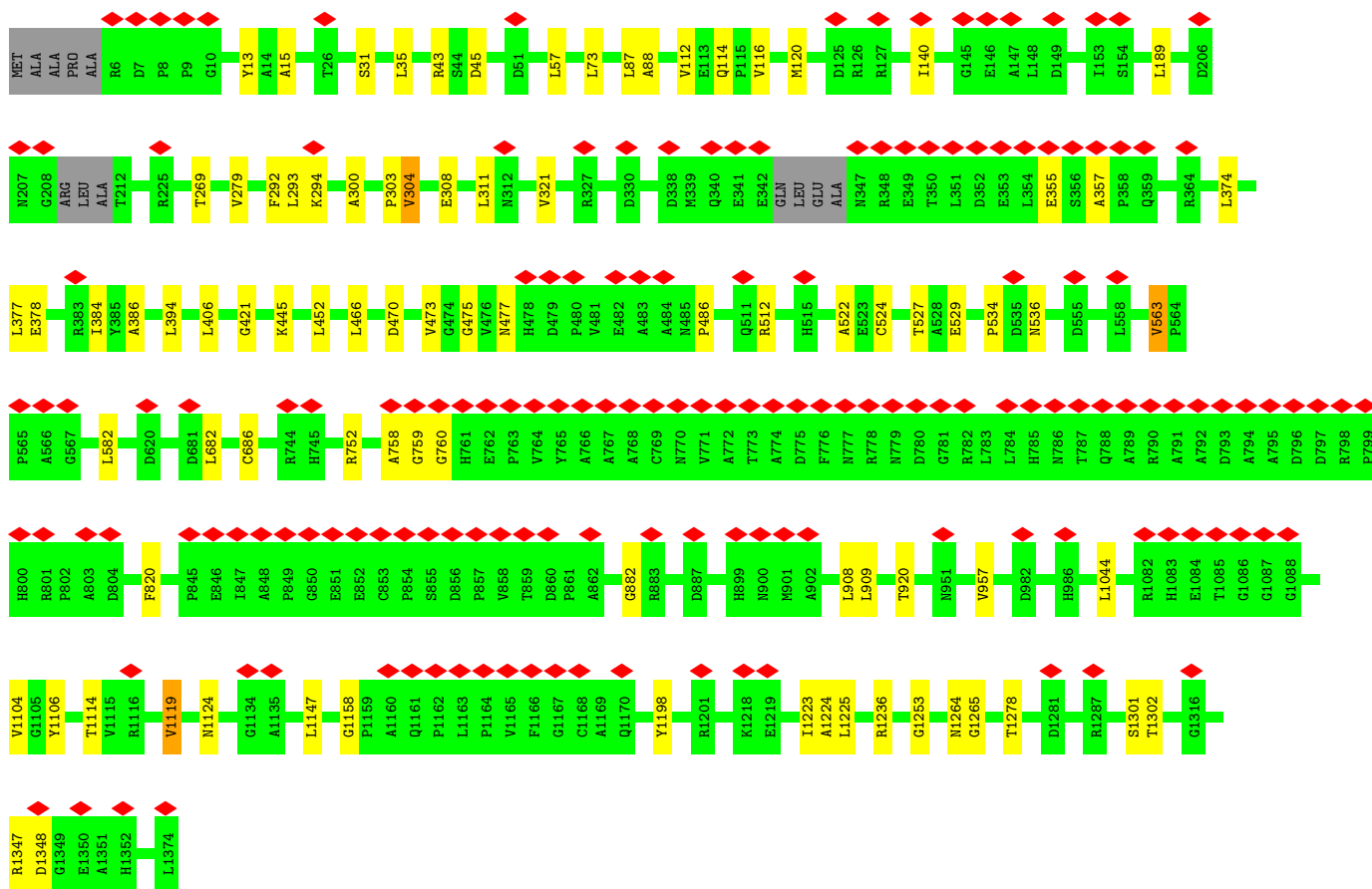
• Molecule 1: Major capsid protein

Chain K: 11% 92% 6% ..

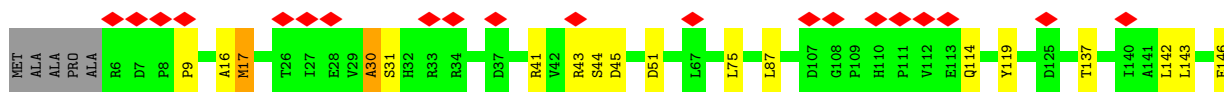




• Molecule 1: Major capsid protein

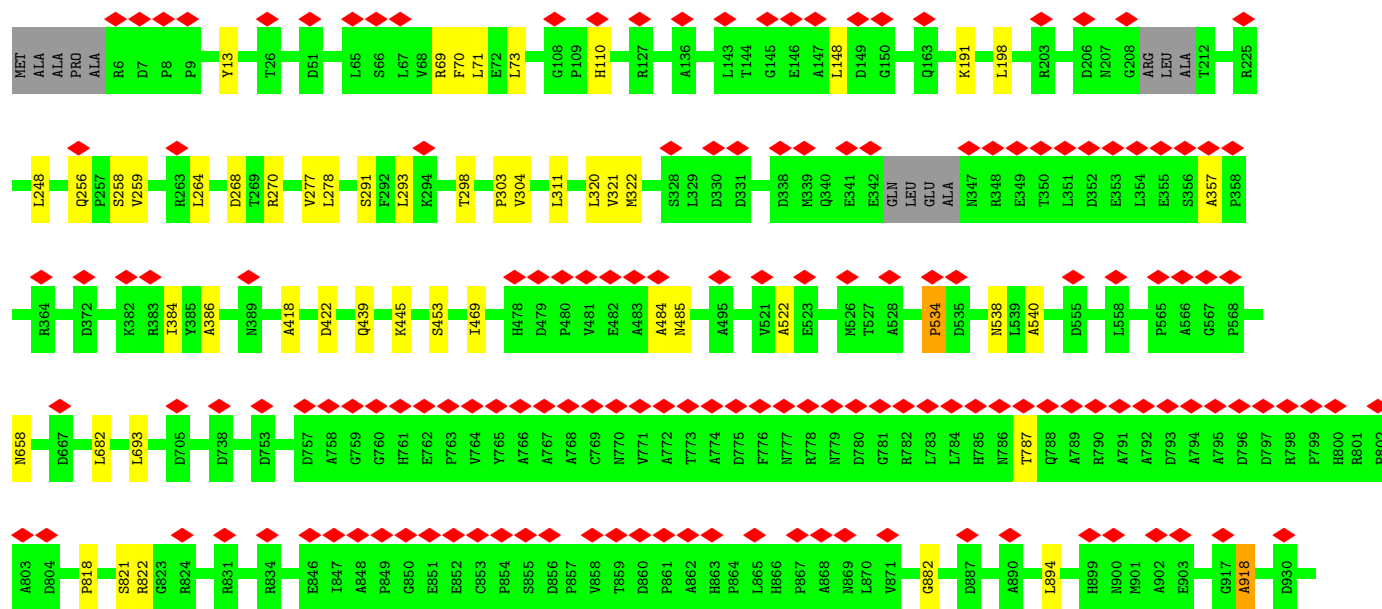
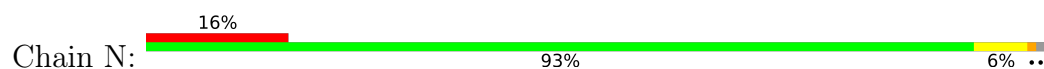


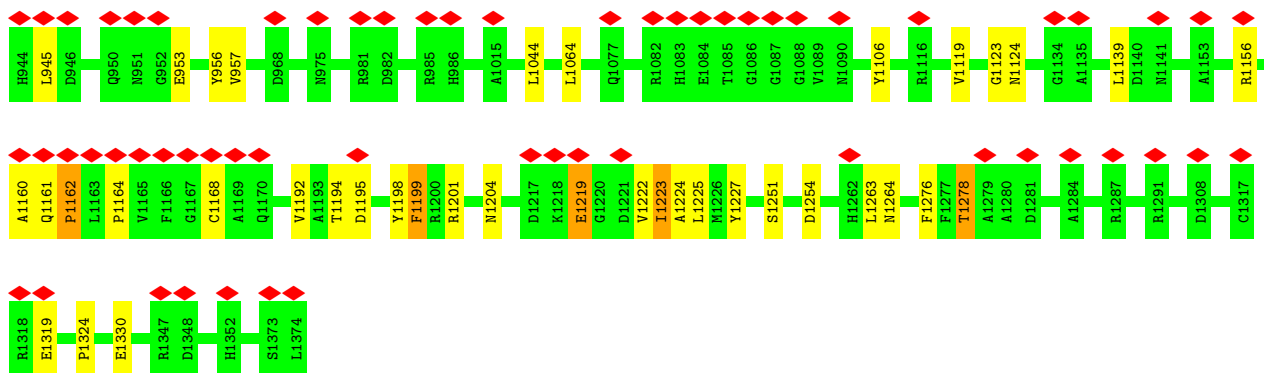
• Molecule 1: Major capsid protein



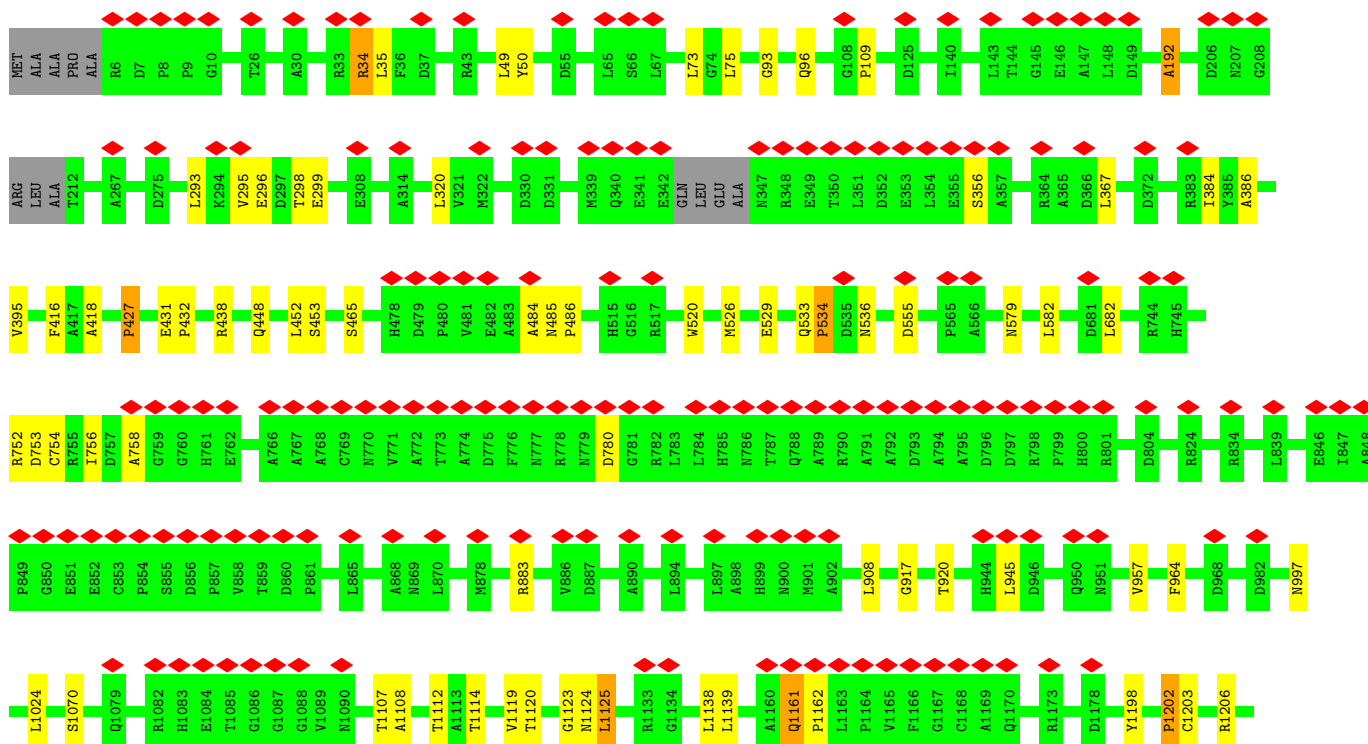


• Molecule 1: Major capsid protein

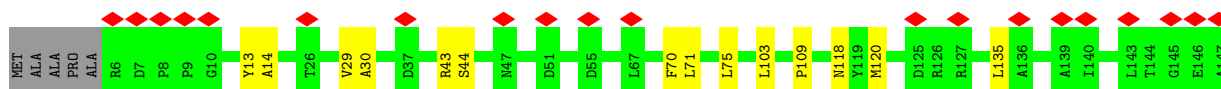


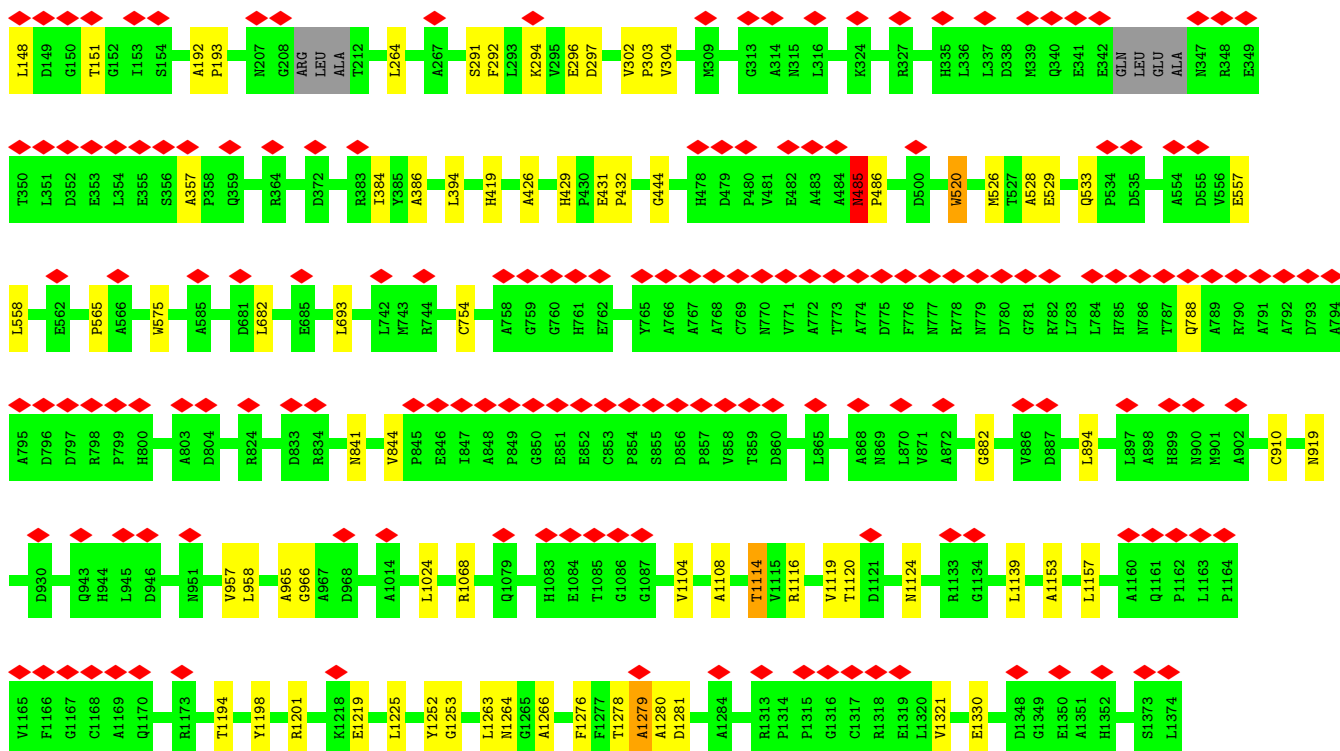


• Molecule 1: Major capsid protein

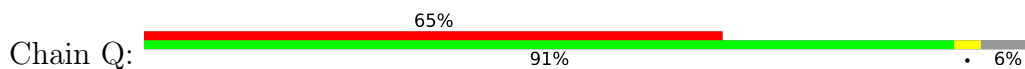


• Molecule 1: Major capsid protein

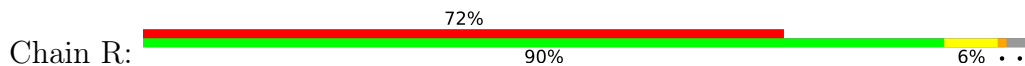


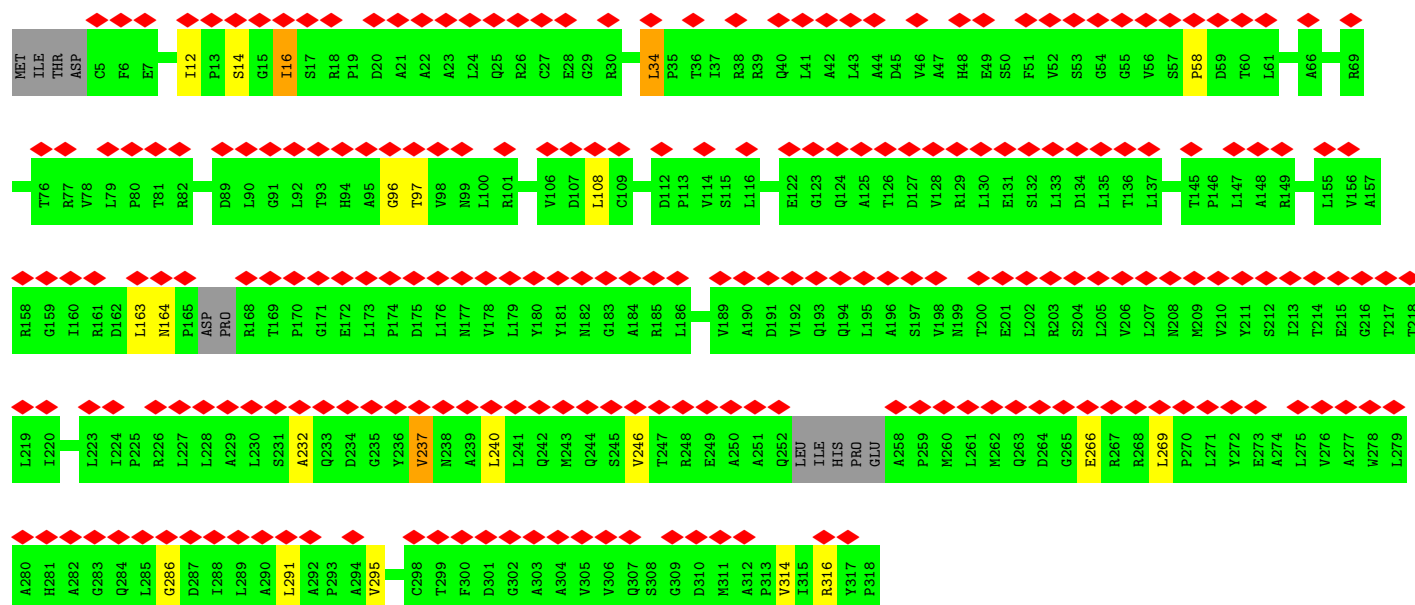


• Molecule 2: Triplex capsid protein 2



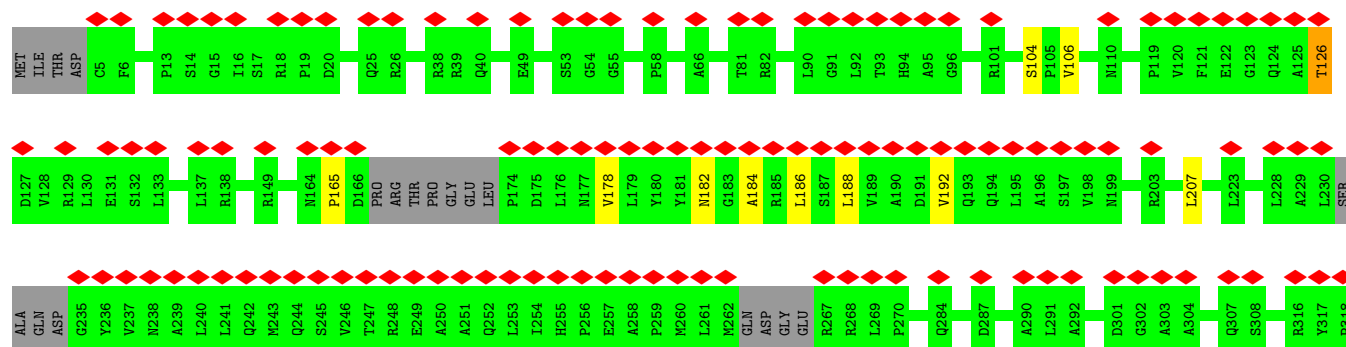
• Molecule 2: Triplex capsid protein 2





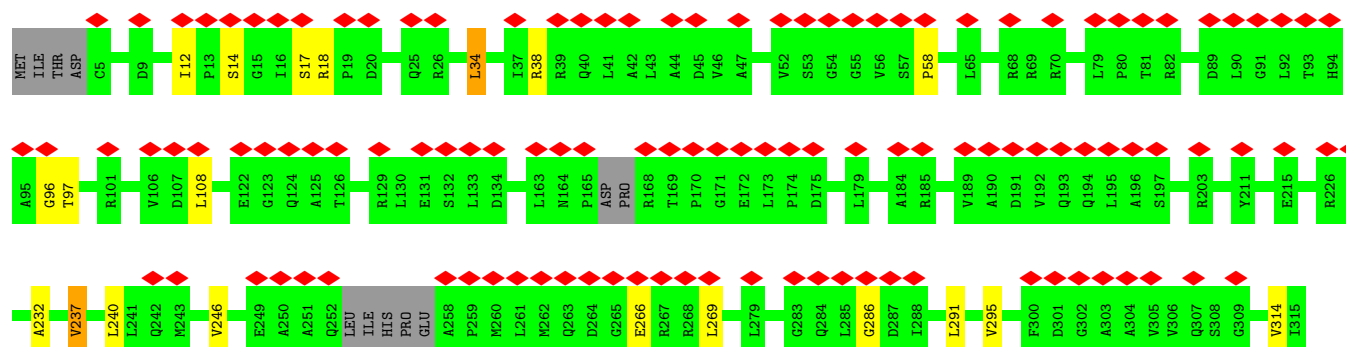
• Molecule 2: Triplex capsid protein 2

Chain T: 40% 91% 6%



• Molecule 2: Triplex capsid protein 2

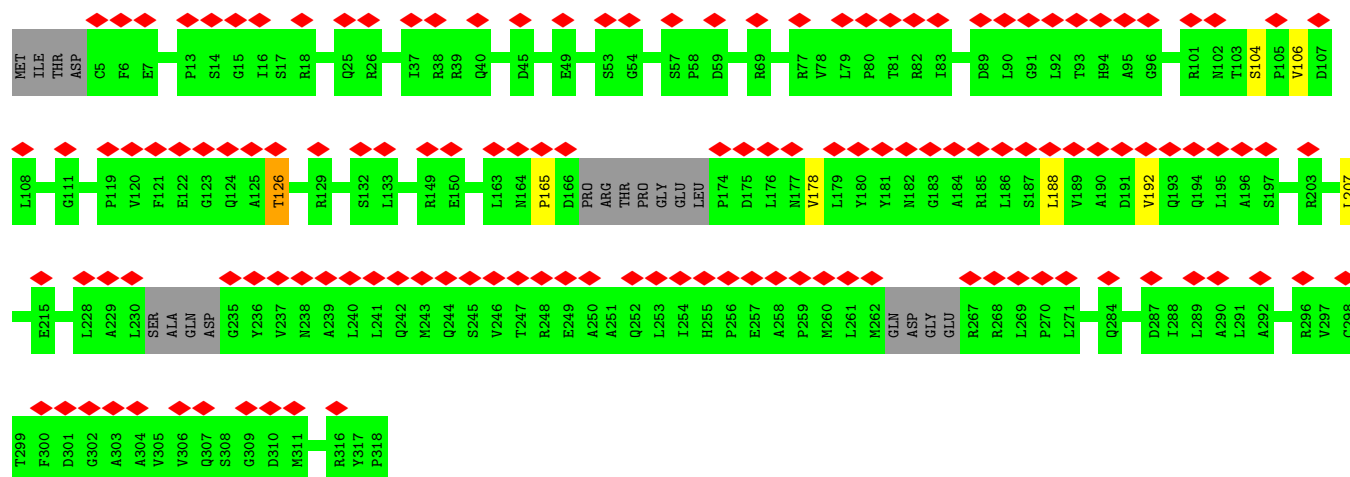
Chain U: 37% 90% 6%





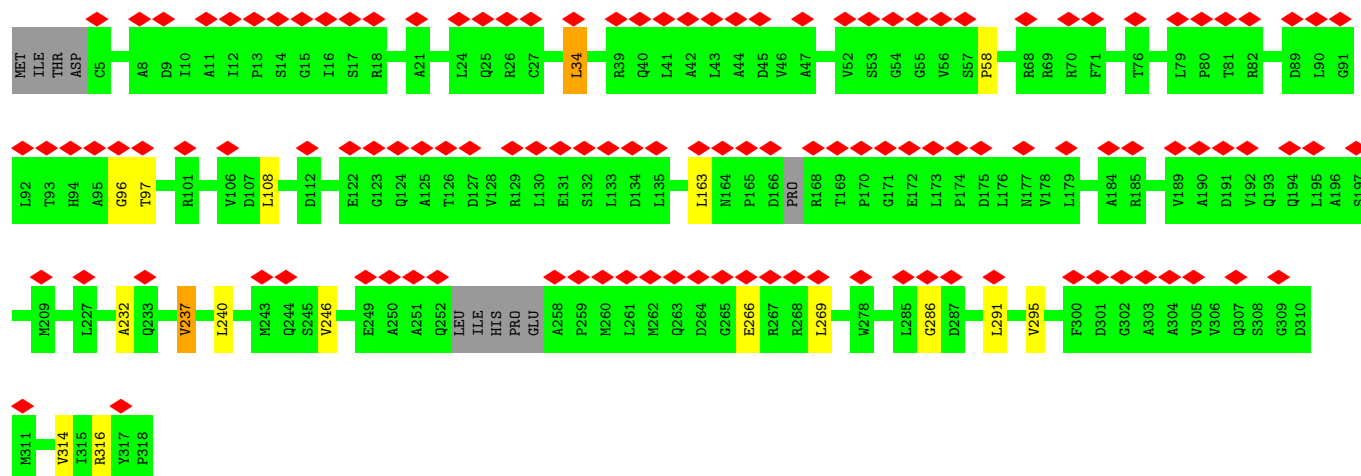
• Molecule 2: Triplex capsid protein 2

Chain W: 42% 92% 6%



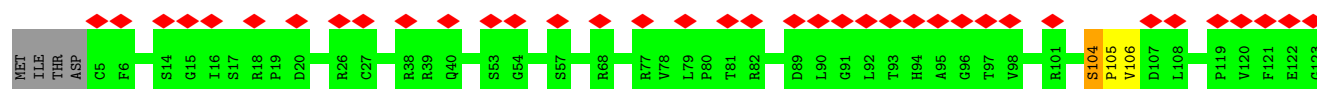
• Molecule 2: Triplex capsid protein 2

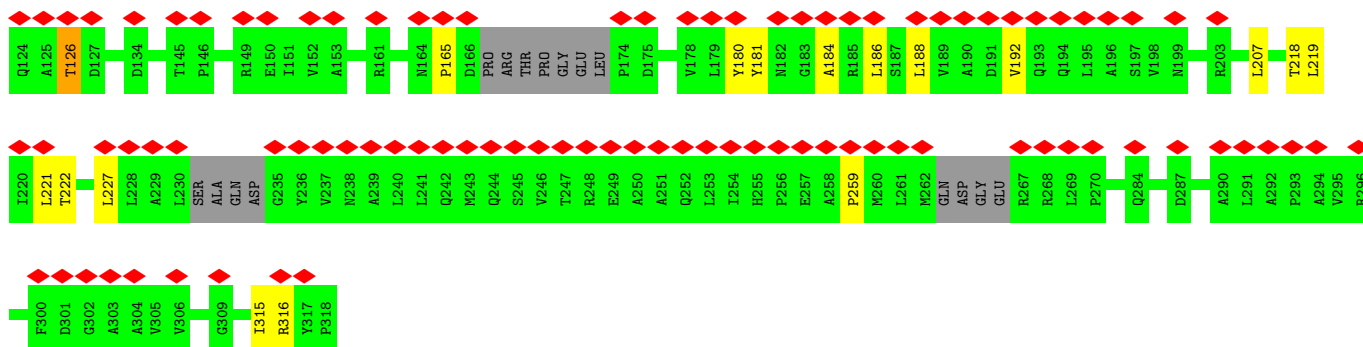
Chain X: 39% 92% 5%



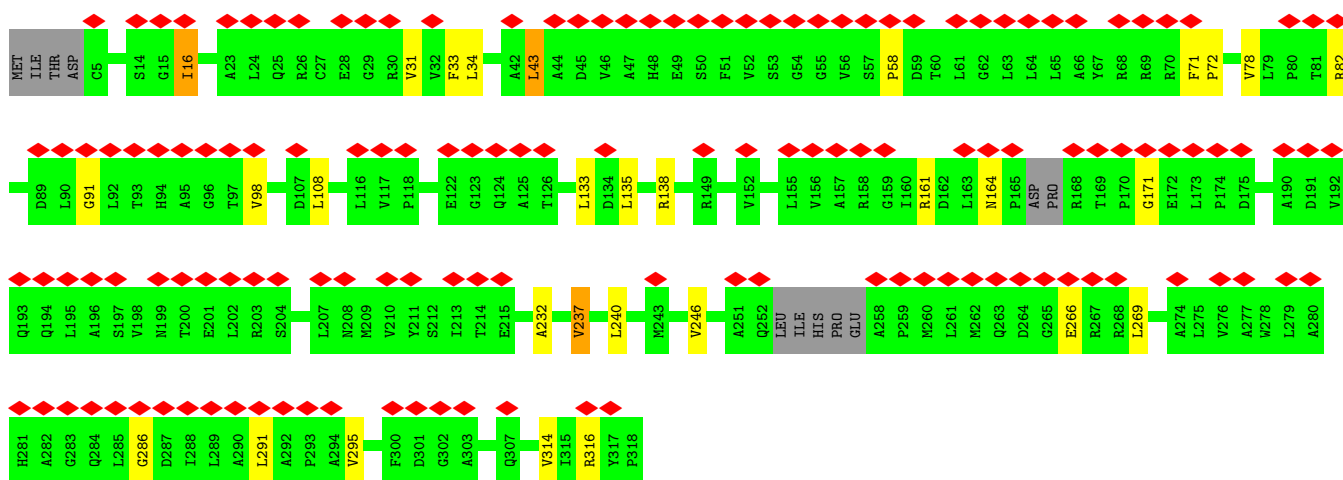
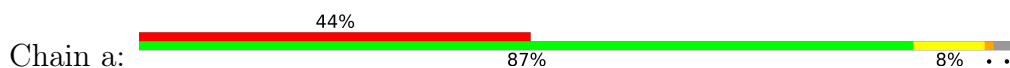
• Molecule 2: Triplex capsid protein 2

Chain Z: 41% 88% 6%

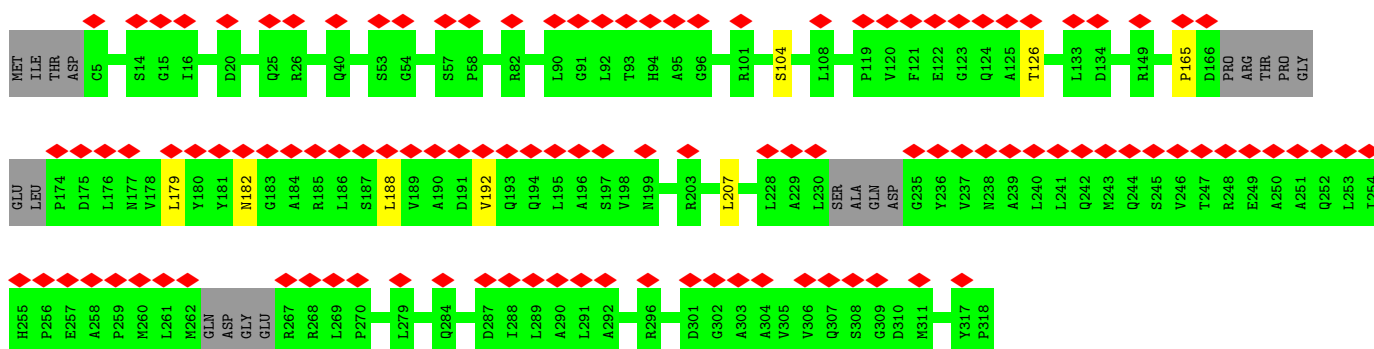
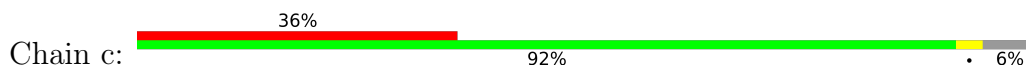




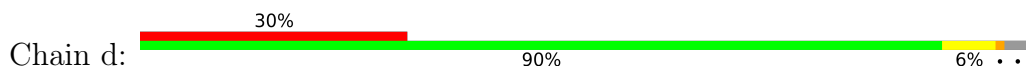
• Molecule 2: Triplex capsid protein 2

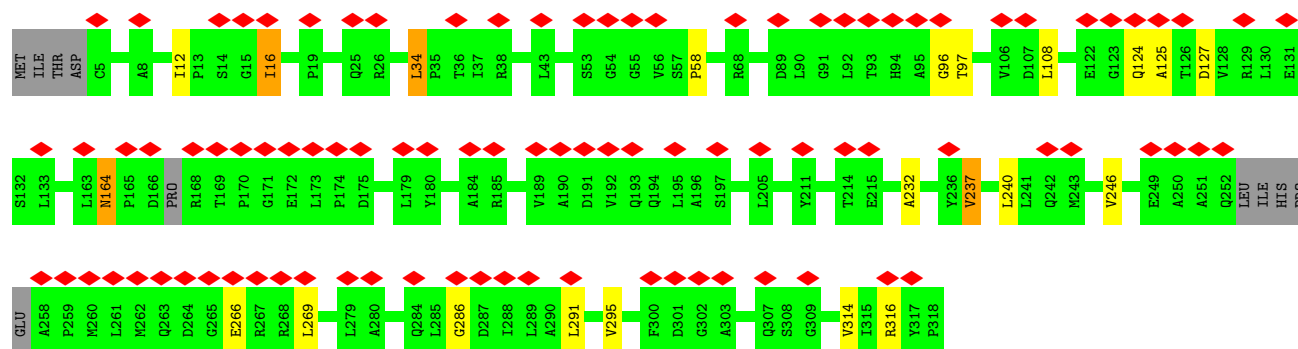


• Molecule 2: Triplex capsid protein 2

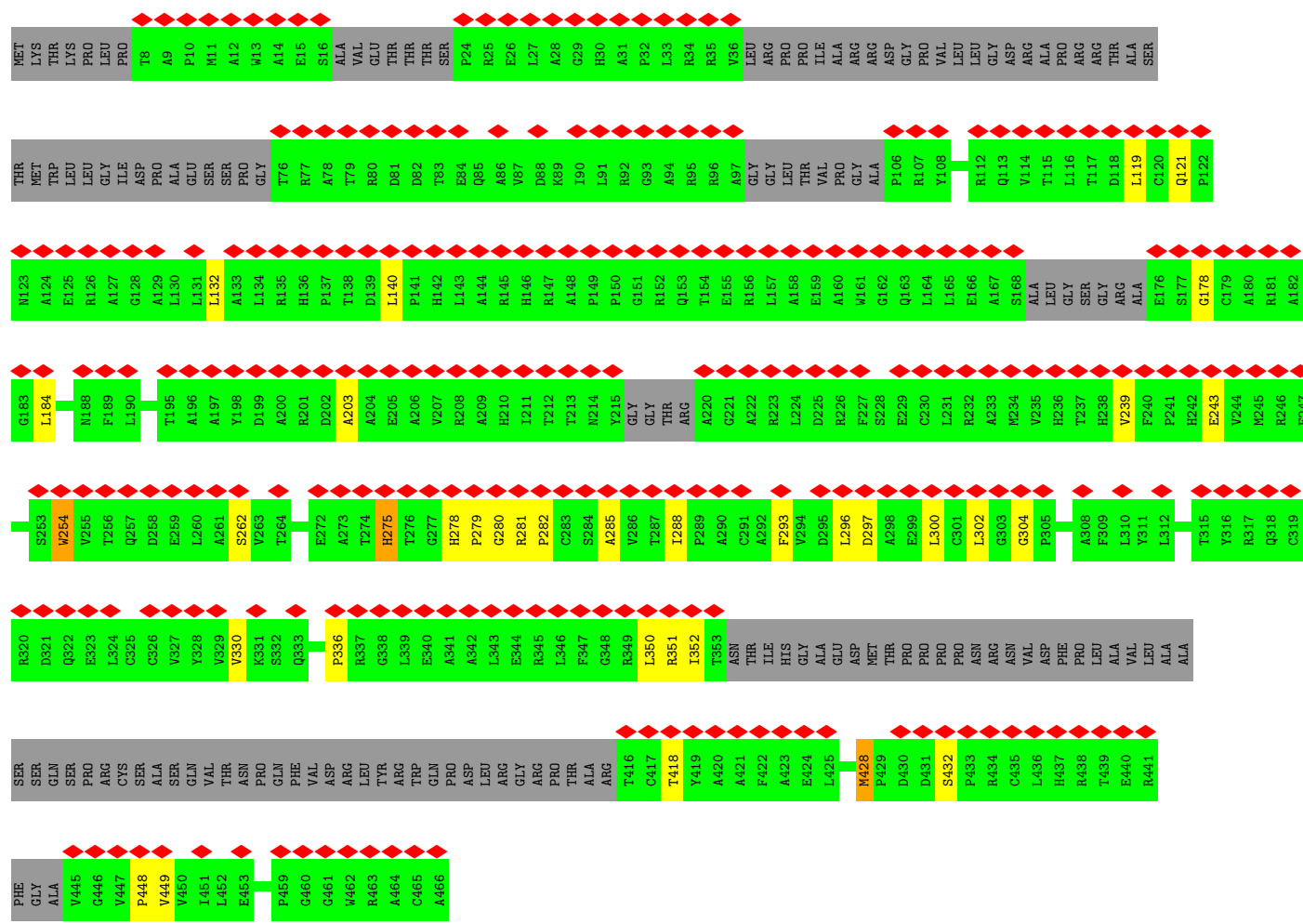


• Molecule 2: Triplex capsid protein 2

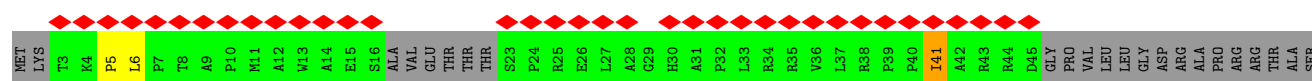


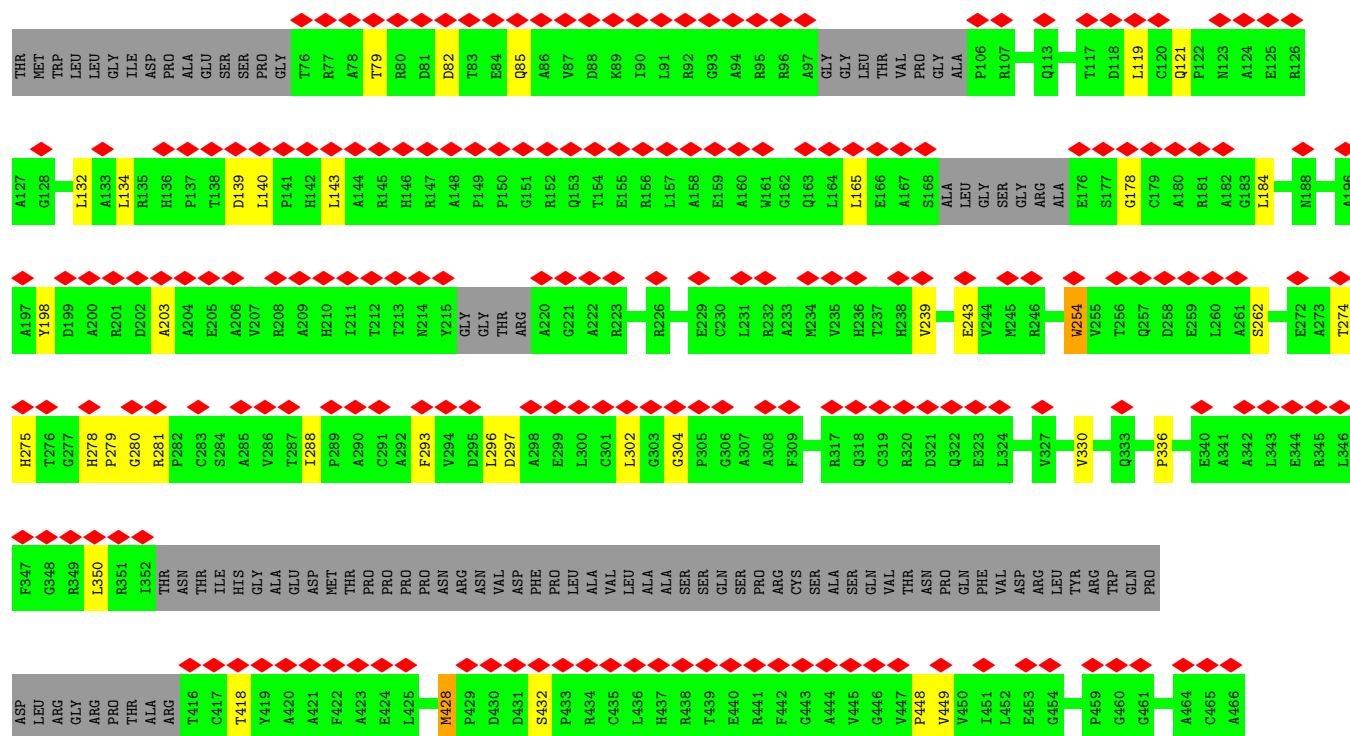


• Molecule 3: Triplex capsid protein 1

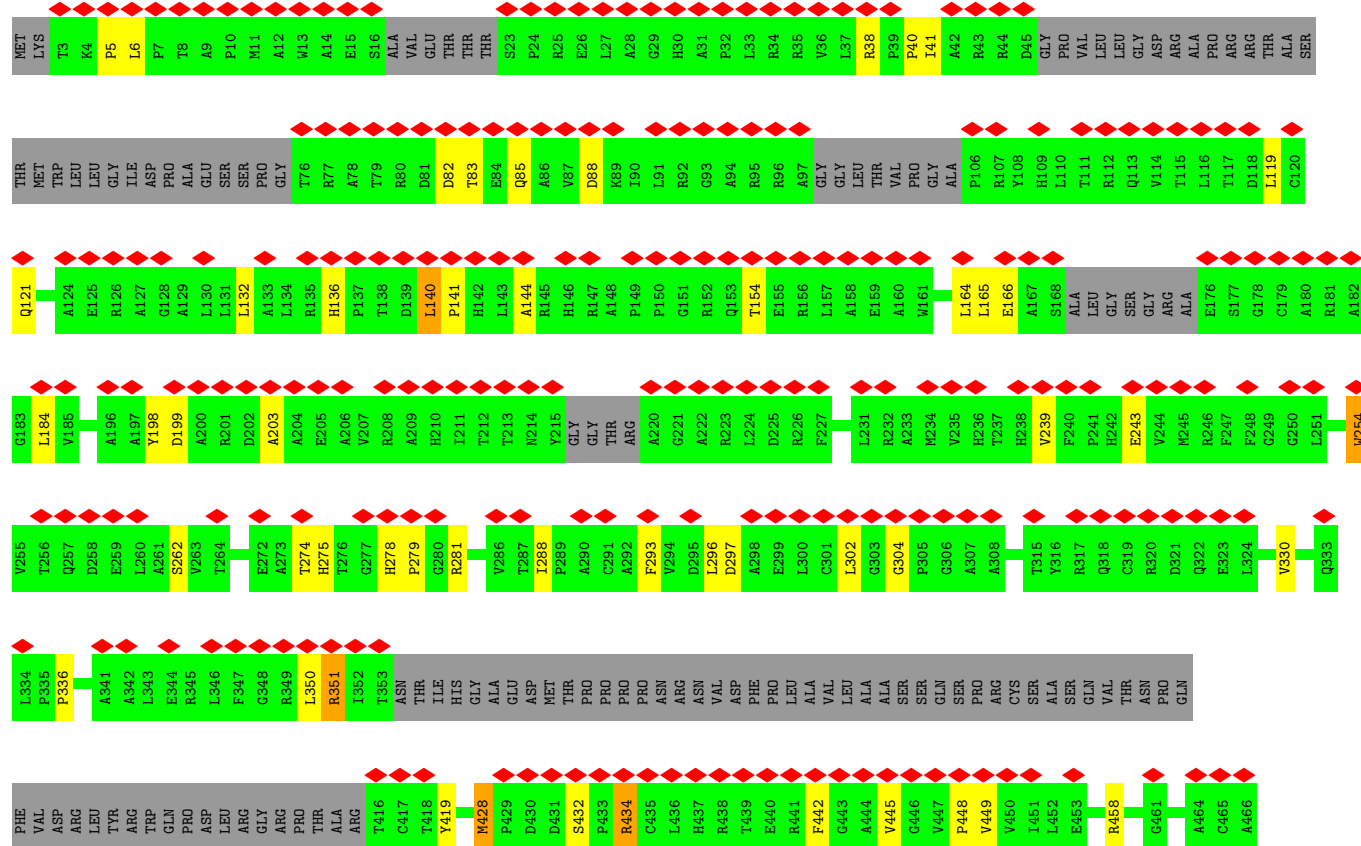


• Molecule 3: Triplex capsid protein 1

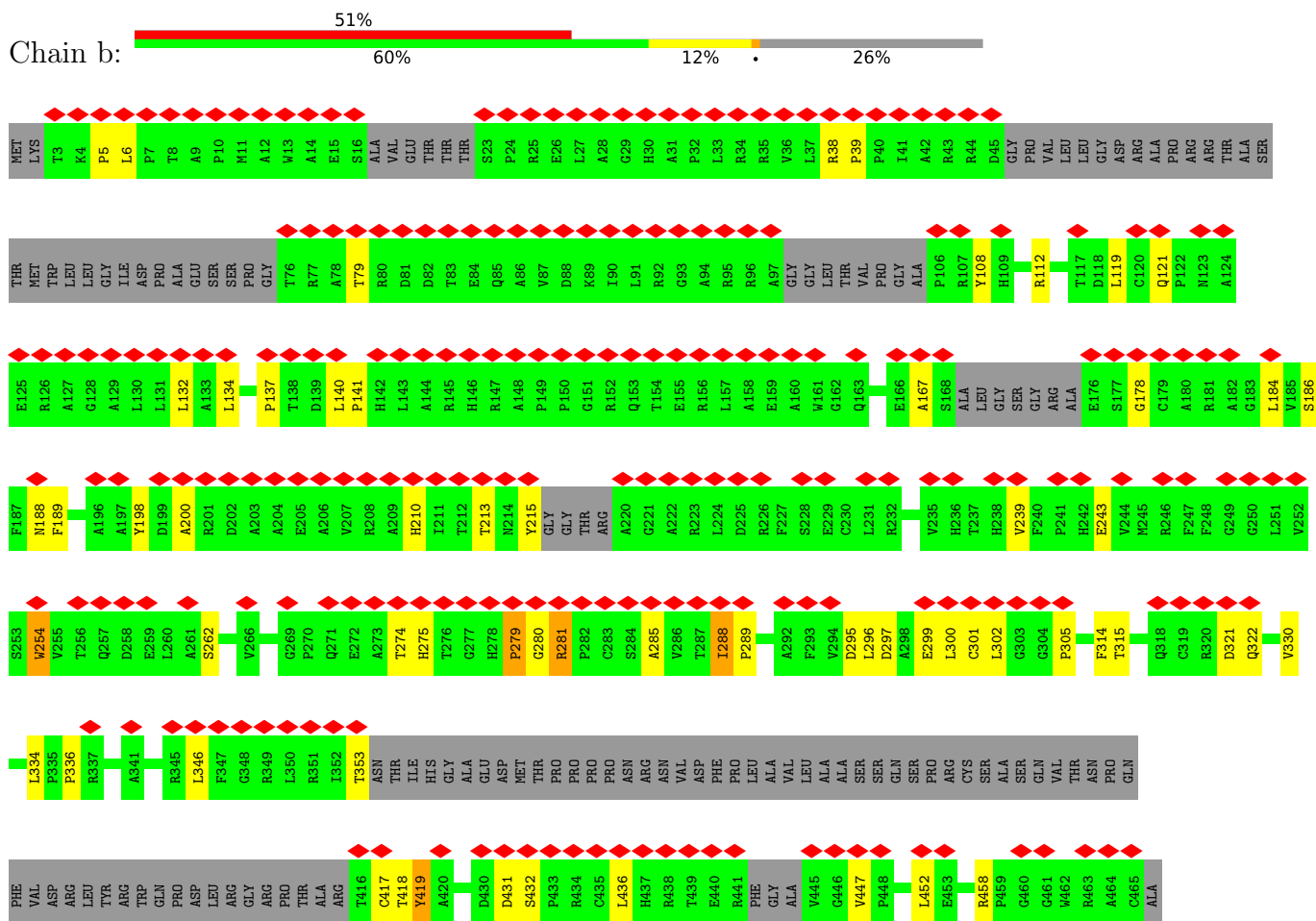




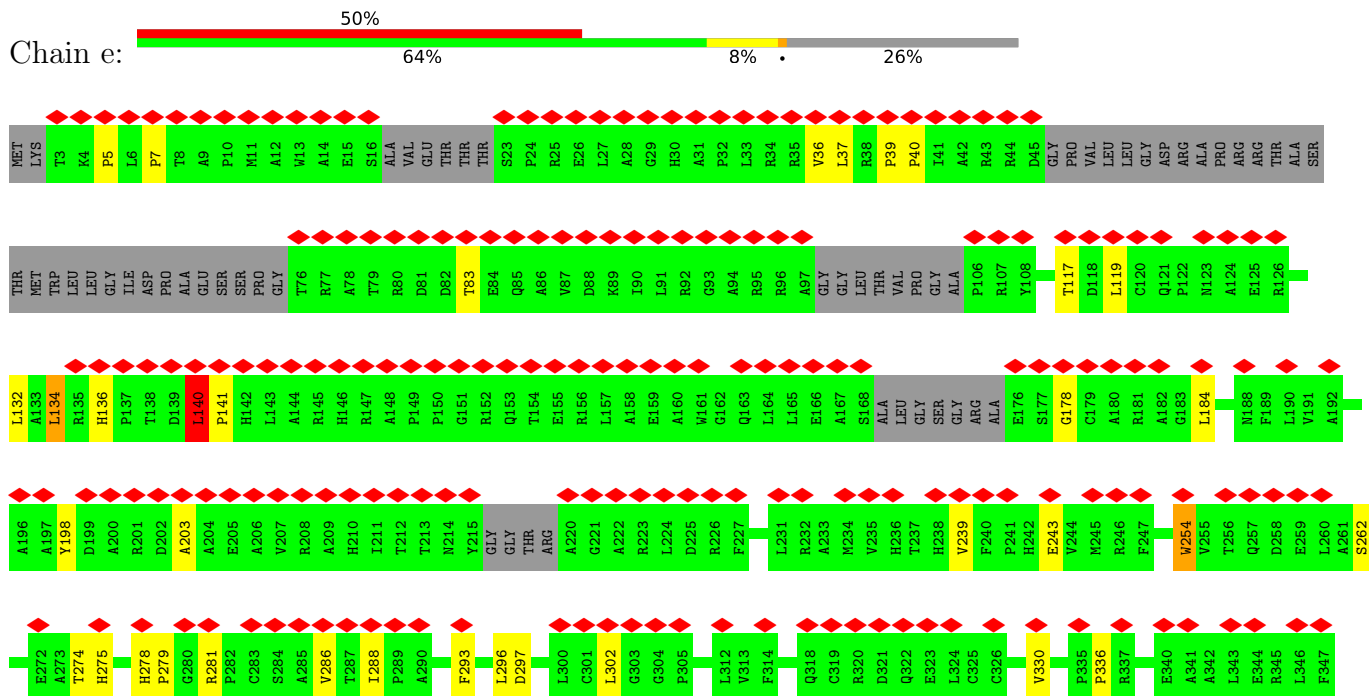
### • Molecule 3: Triplex capsid protein 1

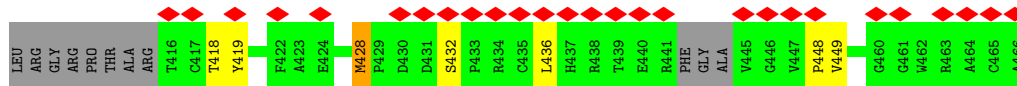
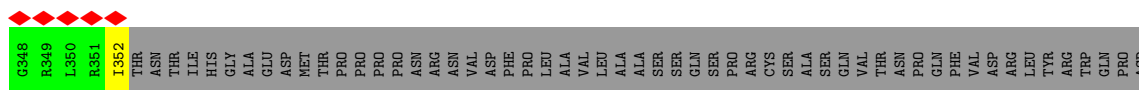


Chain b:

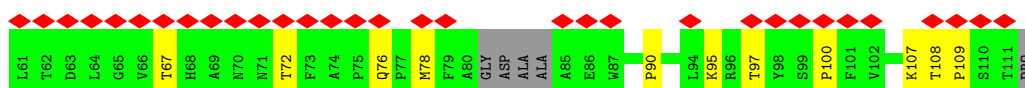
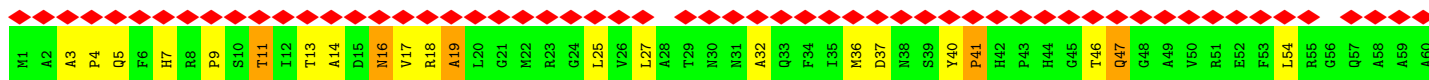
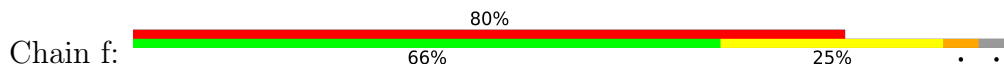


## Chain e:

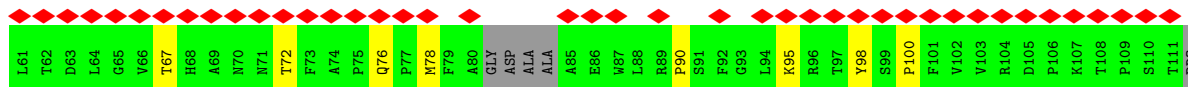
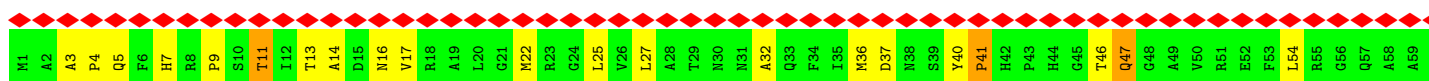
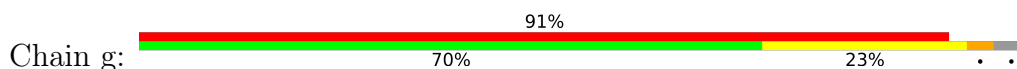




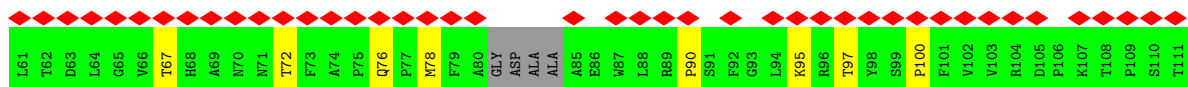
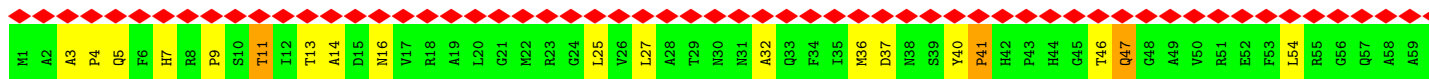
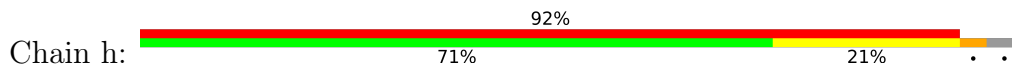
• Molecule 4: Small capsomere-interacting protein



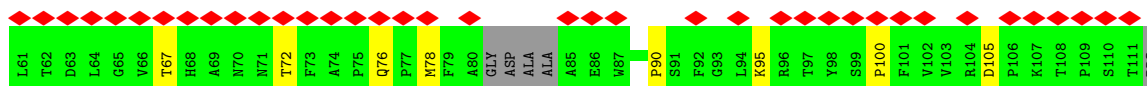
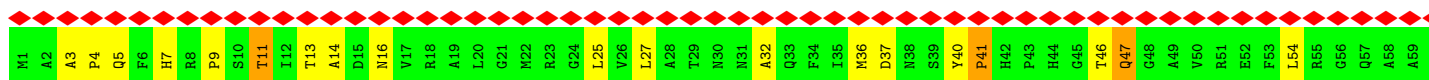
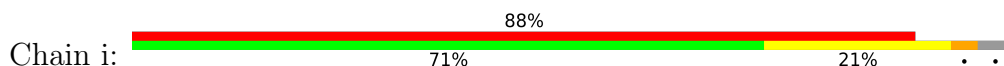
• Molecule 4: Small capsomere-interacting protein



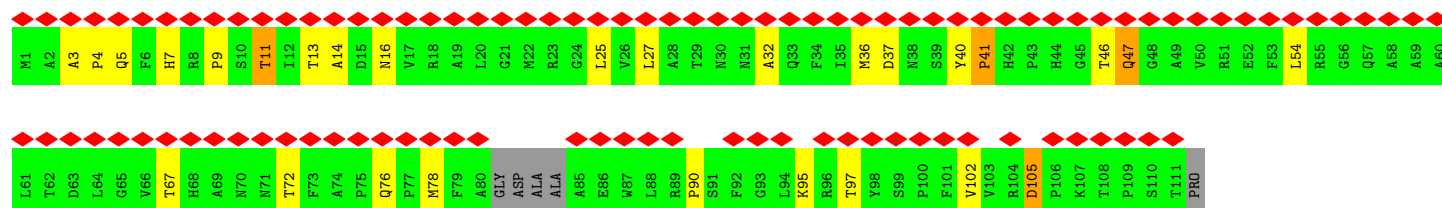
• Molecule 4: Small capsomere-interacting protein



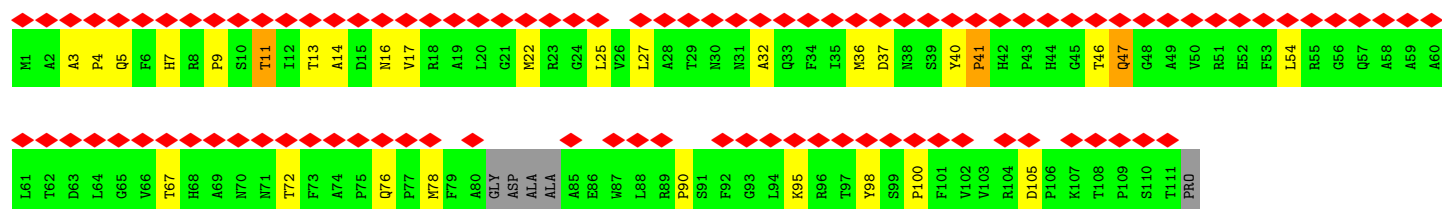
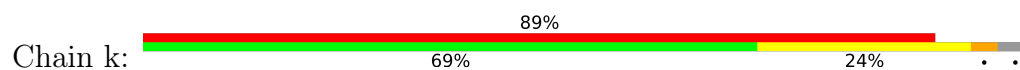
• Molecule 4: Small capsomere-interacting protein



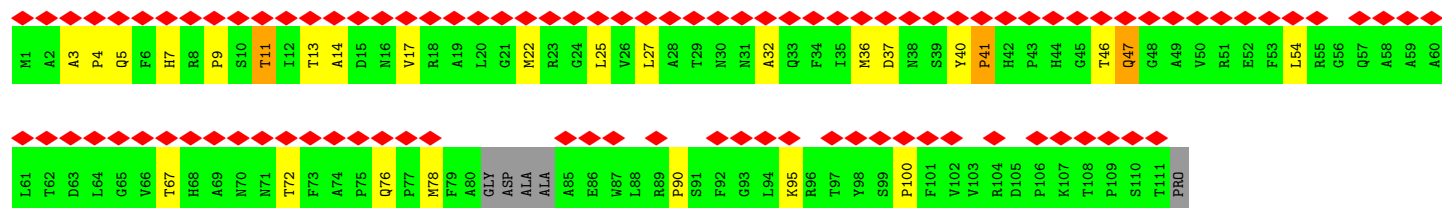
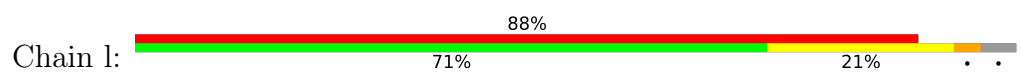
## • Molecule 4: Small capsomere-interacting protein



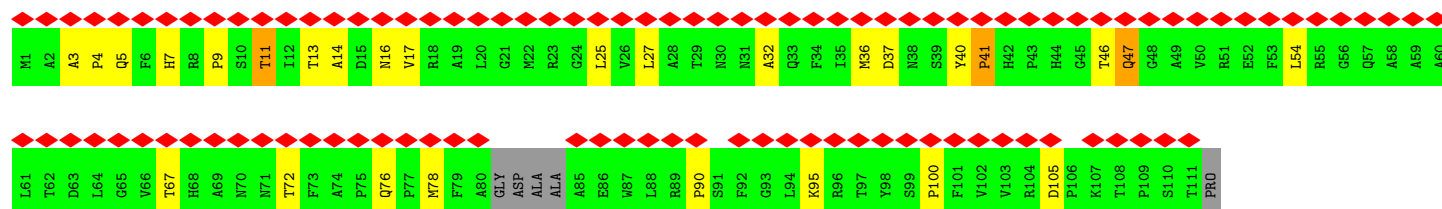
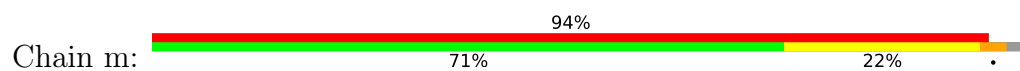
## • Molecule 4: Small capsomere-interacting protein



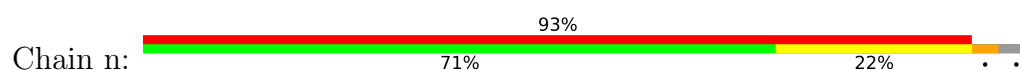
## • Molecule 4: Small capsomere-interacting protein

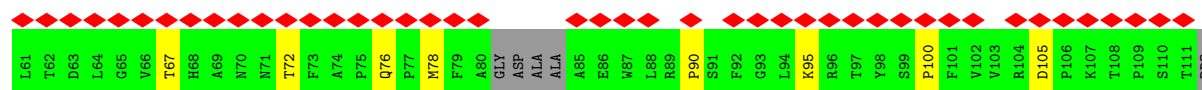


## • Molecule 4: Small capsomere-interacting protein

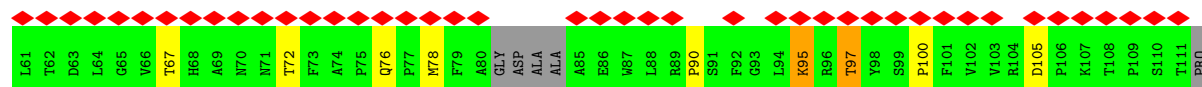


## • Molecule 4: Small capsomere-interacting protein

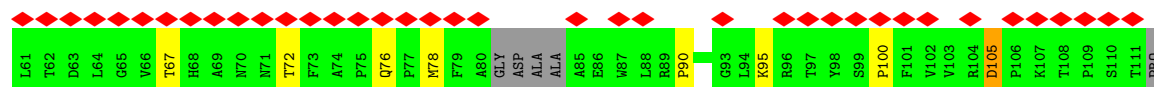
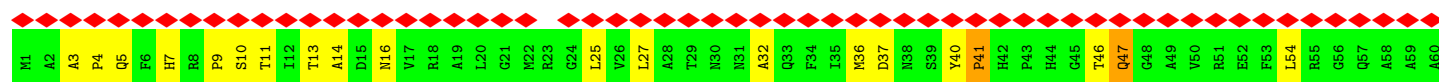
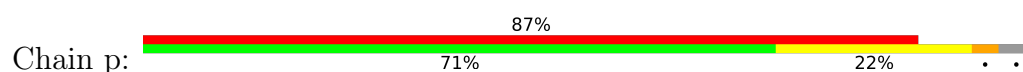




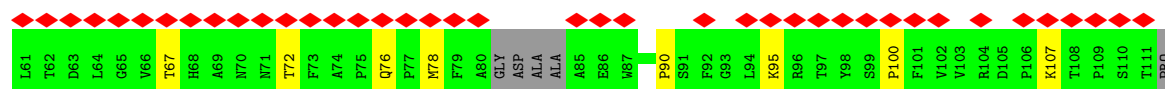
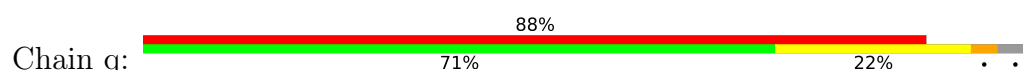
• Molecule 4: Small capsomere-interacting protein



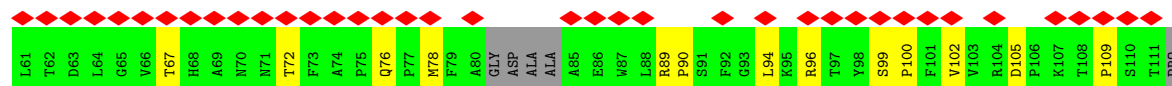
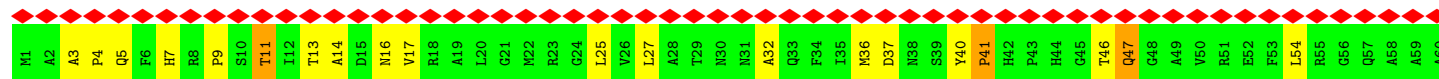
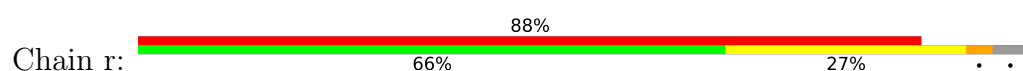
• Molecule 4: Small capsomere-interacting protein



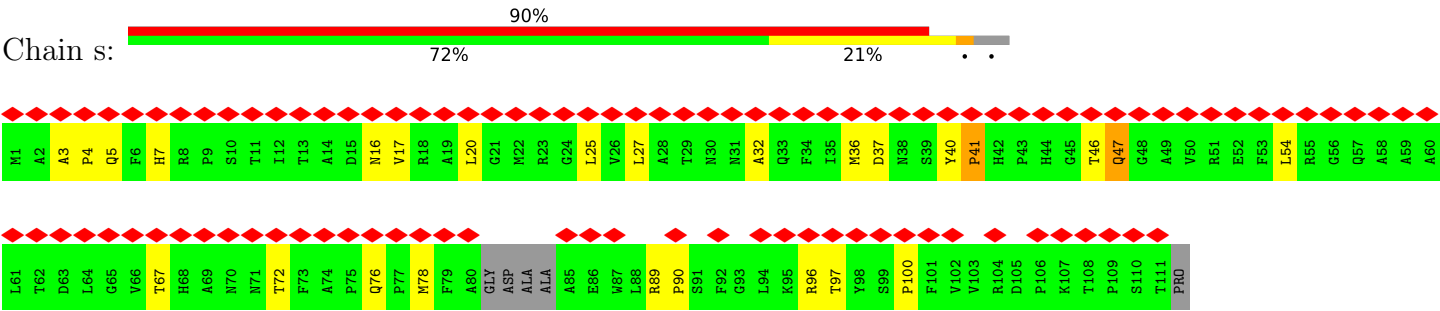
• Molecule 4: Small capsomere-interacting protein



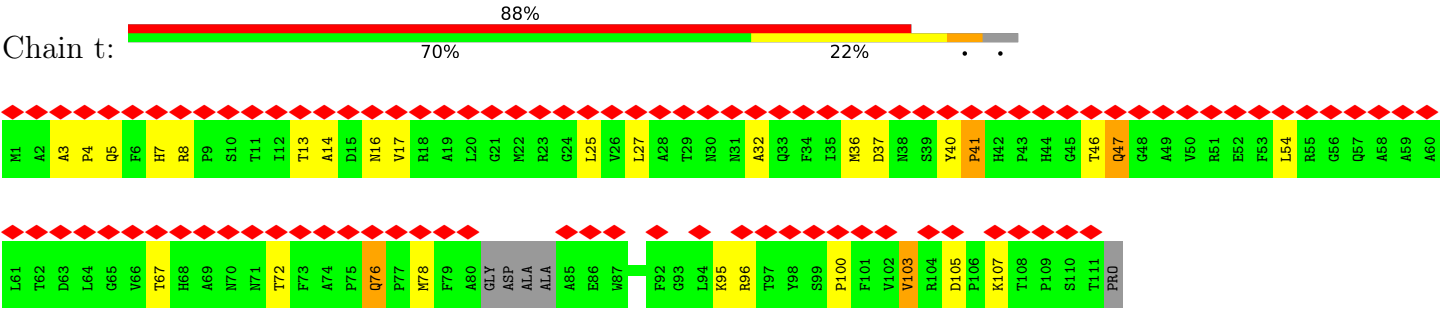
• Molecule 4: Small capsomere-interacting protein



• Molecule 4: Small capsomere-interacting protein



• Molecule 4: Small capsomere-interacting protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	121.639	Depositor
Minimum map value	-84.361	Depositor
Average map value	0.001	Depositor
Map value standard deviation	3.240	Depositor
Recommended contour level	12	Depositor
Map size ( $\text{\AA}$ )	1656.0, 1656.0, 1656.0	wwPDB
Map dimensions	1200, 1200, 1200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.38, 1.38, 1.38	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	0.65	1/10414 (0.0%)	0.85	33/14248 (0.2%)
1	B	0.68	0/10355	0.84	32/14158 (0.2%)
1	C	0.69	0/10476	0.84	27/14321 (0.2%)
1	D	0.63	1/10485 (0.0%)	0.81	28/14333 (0.2%)
1	E	0.61	0/10488	0.80	27/14335 (0.2%)
1	F	0.69	3/10494 (0.0%)	0.81	20/14341 (0.1%)
1	G	0.59	1/10355 (0.0%)	0.87	43/14175 (0.3%)
1	H	0.60	1/10501 (0.0%)	0.79	20/14351 (0.1%)
1	I	0.72	0/10495	0.87	30/14343 (0.2%)
1	J	0.79	1/10460 (0.0%)	0.97	53/14301 (0.4%)
1	K	1.01	6/10509 (0.1%)	1.00	58/14360 (0.4%)
1	L	0.99	8/10497 (0.1%)	1.00	50/14346 (0.3%)
1	M	0.93	11/10532 (0.1%)	0.99	68/14394 (0.5%)
1	N	0.90	9/10509 (0.1%)	0.98	59/14360 (0.4%)
1	O	1.00	7/10507 (0.1%)	1.00	58/14358 (0.4%)
1	P	0.96	7/10512 (0.1%)	0.97	54/14365 (0.4%)
2	Q	0.67	0/2114	0.84	3/2909 (0.1%)
2	R	0.65	0/2215	0.94	10/3047 (0.3%)
2	T	0.69	0/2114	0.84	3/2909 (0.1%)
2	U	0.65	0/2219	0.93	10/3052 (0.3%)
2	W	0.68	0/2114	0.84	3/2909 (0.1%)
2	X	0.64	0/2227	0.92	9/3063 (0.3%)
2	Z	0.69	0/2099	0.86	5/2891 (0.2%)
2	a	0.69	0/2209	1.04	14/3040 (0.5%)
2	c	0.69	0/2114	0.84	1/2909 (0.0%)
2	d	0.65	0/2227	0.96	14/3063 (0.5%)
3	S	0.67	0/2311	1.09	20/3167 (0.6%)
3	V	0.67	0/2413	1.11	24/3309 (0.7%)
3	Y	0.69	0/2433	1.23	27/3334 (0.8%)
3	b	0.64	0/2376	1.06	18/3261 (0.6%)
3	e	0.67	0/2410	1.08	20/3301 (0.6%)
4	f	0.83	1/635 (0.2%)	1.51	14/877 (1.6%)
4	g	0.83	1/635 (0.2%)	1.42	11/877 (1.3%)
4	h	0.81	1/635 (0.2%)	1.40	10/877 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	i	0.82	1/635 (0.2%)	1.41	11/877 (1.3%)
4	j	0.81	1/639 (0.2%)	1.40	11/881 (1.2%)
4	k	0.83	1/635 (0.2%)	1.42	11/877 (1.3%)
4	l	0.82	1/635 (0.2%)	1.40	10/877 (1.1%)
4	m	0.82	1/635 (0.2%)	1.41	11/877 (1.3%)
4	n	0.82	1/632 (0.2%)	1.42	11/874 (1.3%)
4	o	0.82	1/635 (0.2%)	1.43	11/877 (1.3%)
4	p	0.83	1/635 (0.2%)	1.39	11/877 (1.3%)
4	q	0.84	1/635 (0.2%)	1.43	10/877 (1.1%)
4	r	0.77	1/639 (0.2%)	1.45	13/881 (1.5%)
4	s	0.75	1/641 (0.2%)	1.39	8/884 (0.9%)
4	t	0.77	1/635 (0.2%)	1.36	11/877 (1.3%)
All	All	0.77	71/210720 (0.0%)	0.95	1005/288420 (0.3%)

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	2
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
2	R	0	1
2	U	0	1
2	X	0	1
2	a	0	1
2	d	0	1
3	S	0	1
3	V	0	1
3	Y	0	1
3	e	0	1
4	f	0	1
4	g	0	1
4	h	0	1
4	i	0	1
4	j	0	1
4	k	0	1
4	l	0	1
4	m	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
4	n	0	1
4	o	0	1
4	p	0	1
4	q	0	1
4	r	0	1
4	s	0	1
4	t	0	1
All	All	0	30

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	818	PRO	N-CD	-8.60	1.35	1.47
1	L	1253	GLY	C-O	-8.07	1.10	1.23
1	P	1198	TYR	CE1-CZ	-7.96	1.28	1.38
1	J	273	PRO	N-CD	-7.86	1.36	1.47
1	F	818	PRO	N-CD	-7.84	1.36	1.47

The worst 5 of 1005 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	140	LEU	C-N-CD	-29.80	55.04	120.60
1	M	1161	GLN	C-N-CD	-13.85	90.14	120.60
3	e	140	LEU	C-N-CD	-11.74	94.77	120.60
3	b	281	ARG	C-N-CD	-11.72	94.82	120.60
1	L	1265	GLY	N-CA-C	-11.18	85.14	113.10

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1276	PHE	Mainchain
1	A	374	LEU	Mainchain
1	B	265	THR	Mainchain
1	C	464	PRO	Mainchain
1	D	92	GLU	Mainchain

## 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 ⓘ

### 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	1363/1374 (99%)	1209 (89%)	140 (10%)	14 (1%)	13	42
1	B	1344/1374 (98%)	1194 (89%)	129 (10%)	21 (2%)	8	31
1	C	1356/1374 (99%)	1212 (89%)	126 (9%)	18 (1%)	10	36
1	D	1356/1374 (99%)	1212 (89%)	124 (9%)	20 (2%)	8	33
1	E	1356/1374 (99%)	1201 (89%)	143 (10%)	12 (1%)	14	45
1	F	1356/1374 (99%)	1212 (89%)	125 (9%)	19 (1%)	9	34
1	G	1363/1374 (99%)	1193 (88%)	148 (11%)	22 (2%)	8	31
1	H	1356/1374 (99%)	1220 (90%)	123 (9%)	13 (1%)	13	42
1	I	1355/1374 (99%)	1228 (91%)	112 (8%)	15 (1%)	12	39
1	J	1356/1374 (99%)	1206 (89%)	132 (10%)	18 (1%)	10	36
1	K	1356/1374 (99%)	1235 (91%)	107 (8%)	14 (1%)	13	42
1	L	1356/1374 (99%)	1226 (90%)	114 (8%)	16 (1%)	11	38
1	M	1361/1374 (99%)	1228 (90%)	112 (8%)	21 (2%)	8	33
1	N	1356/1374 (99%)	1218 (90%)	118 (9%)	20 (2%)	8	33
1	O	1356/1374 (99%)	1216 (90%)	121 (9%)	19 (1%)	9	34
1	P	1356/1374 (99%)	1227 (90%)	112 (8%)	17 (1%)	10	36
2	Q	291/318 (92%)	254 (87%)	34 (12%)	3 (1%)	13	42
2	R	301/318 (95%)	264 (88%)	32 (11%)	5 (2%)	7	30
2	T	291/318 (92%)	252 (87%)	34 (12%)	5 (2%)	7	30
2	U	301/318 (95%)	262 (87%)	35 (12%)	4 (1%)	10	36
2	W	291/318 (92%)	254 (87%)	34 (12%)	3 (1%)	13	42
2	X	302/318 (95%)	260 (86%)	39 (13%)	3 (1%)	13	42
2	Z	291/318 (92%)	252 (87%)	33 (11%)	6 (2%)	5	25
2	a	301/318 (95%)	273 (91%)	25 (8%)	3 (1%)	13	42
2	c	291/318 (92%)	254 (87%)	34 (12%)	3 (1%)	13	42

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	d	302/318 (95%)	263 (87%)	34 (11%)	5 (2%)	7	30
3	S	313/466 (67%)	268 (86%)	36 (12%)	9 (3%)	3	20
3	V	332/466 (71%)	278 (84%)	46 (14%)	8 (2%)	5	22
3	Y	333/466 (72%)	276 (83%)	43 (13%)	14 (4%)	2	13
3	b	327/466 (70%)	273 (84%)	37 (11%)	17 (5%)	1	10
3	e	327/466 (70%)	265 (81%)	47 (14%)	15 (5%)	2	12
4	f	103/112 (92%)	70 (68%)	15 (15%)	18 (18%)	0	0
4	g	103/112 (92%)	71 (69%)	17 (16%)	15 (15%)	0	0
4	h	103/112 (92%)	73 (71%)	17 (16%)	13 (13%)	0	1
4	i	103/112 (92%)	73 (71%)	17 (16%)	13 (13%)	0	1
4	j	103/112 (92%)	71 (69%)	17 (16%)	15 (15%)	0	0
4	k	103/112 (92%)	71 (69%)	16 (16%)	16 (16%)	0	0
4	l	103/112 (92%)	70 (68%)	19 (18%)	14 (14%)	0	1
4	m	103/112 (92%)	71 (69%)	18 (18%)	14 (14%)	0	1
4	n	103/112 (92%)	71 (69%)	19 (18%)	13 (13%)	0	1
4	o	103/112 (92%)	70 (68%)	17 (16%)	16 (16%)	0	0
4	p	103/112 (92%)	74 (72%)	16 (16%)	13 (13%)	0	1
4	q	103/112 (92%)	71 (69%)	17 (16%)	15 (15%)	0	0
4	r	103/112 (92%)	70 (68%)	16 (16%)	17 (16%)	0	0
4	s	103/112 (92%)	77 (75%)	13 (13%)	13 (13%)	0	1
4	t	103/112 (92%)	75 (73%)	12 (12%)	16 (16%)	0	0
All	All	27841/29174 (95%)	24463 (88%)	2775 (10%)	603 (2%)	8	24

5 of 603 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	137	THR
1	G	295	VAL
1	G	1223	ILE
1	G	1277	PHE
1	G	1278	THR

### 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	1003/1080 (93%)	983 (98%)	20 (2%)	50	74
1	B	1009/1080 (93%)	991 (98%)	18 (2%)	54	76
1	C	1020/1080 (94%)	1008 (99%)	12 (1%)	67	83
1	D	1023/1080 (95%)	1000 (98%)	23 (2%)	47	71
1	E	1023/1080 (95%)	1009 (99%)	14 (1%)	62	81
1	F	1024/1080 (95%)	1005 (98%)	19 (2%)	52	75
1	G	992/1080 (92%)	964 (97%)	28 (3%)	38	66
1	H	1027/1080 (95%)	1009 (98%)	18 (2%)	54	76
1	I	1027/1080 (95%)	1001 (98%)	26 (2%)	42	69
1	J	1016/1080 (94%)	995 (98%)	21 (2%)	48	72
1	K	1028/1080 (95%)	1001 (97%)	27 (3%)	41	68
1	L	1027/1080 (95%)	1005 (98%)	22 (2%)	48	72
1	M	1030/1080 (95%)	1005 (98%)	25 (2%)	44	70
1	N	1029/1080 (95%)	1016 (99%)	13 (1%)	65	82
1	O	1027/1080 (95%)	1006 (98%)	21 (2%)	50	74
1	P	1029/1080 (95%)	1007 (98%)	22 (2%)	48	72
2	Q	195/264 (74%)	192 (98%)	3 (2%)	60	80
2	R	214/264 (81%)	205 (96%)	9 (4%)	25	56
2	T	195/264 (74%)	191 (98%)	4 (2%)	48	72
2	U	215/264 (81%)	206 (96%)	9 (4%)	25	56
2	W	195/264 (74%)	192 (98%)	3 (2%)	60	80
2	X	216/264 (82%)	209 (97%)	7 (3%)	34	63
2	Z	192/264 (73%)	181 (94%)	11 (6%)	17	46
2	a	213/264 (81%)	197 (92%)	16 (8%)	11	36
2	c	195/264 (74%)	191 (98%)	4 (2%)	48	72
2	d	216/264 (82%)	208 (96%)	8 (4%)	29	59

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	198/366 (54%)	189 (96%)	9 (4%)	23	53
3	V	201/366 (55%)	187 (93%)	14 (7%)	12	39
3	Y	205/366 (56%)	187 (91%)	18 (9%)	8	30
3	b	198/366 (54%)	165 (83%)	33 (17%)	2	7
3	e	204/366 (56%)	191 (94%)	13 (6%)	14	42
4	f	35/88 (40%)	29 (83%)	6 (17%)	1	7
4	g	35/88 (40%)	29 (83%)	6 (17%)	1	7
4	h	35/88 (40%)	28 (80%)	7 (20%)	1	4
4	i	35/88 (40%)	29 (83%)	6 (17%)	1	7
4	j	36/88 (41%)	30 (83%)	6 (17%)	2	7
4	k	35/88 (40%)	29 (83%)	6 (17%)	1	7
4	l	35/88 (40%)	29 (83%)	6 (17%)	1	7
4	m	35/88 (40%)	29 (83%)	6 (17%)	1	7
4	n	34/88 (39%)	27 (79%)	7 (21%)	1	4
4	o	35/88 (40%)	28 (80%)	7 (20%)	1	4
4	p	35/88 (40%)	28 (80%)	7 (20%)	1	4
4	q	35/88 (40%)	29 (83%)	6 (17%)	1	7
4	r	36/88 (41%)	30 (83%)	6 (17%)	2	7
4	s	36/88 (41%)	29 (81%)	7 (19%)	1	5
4	t	35/88 (40%)	29 (83%)	6 (17%)	1	7
All	All	19913/23070 (86%)	19328 (97%)	585 (3%)	39	65

5 of 585 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	447	VAL
4	s	36	MET
2	d	314	VAL
3	b	436	LEU
4	j	67	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 537 such sidechains are listed below:

Mol	Chain	Res	Type
3	V	242	HIS
3	Y	136	HIS
3	V	238	HIS
4	j	7	HIS
1	H	696	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

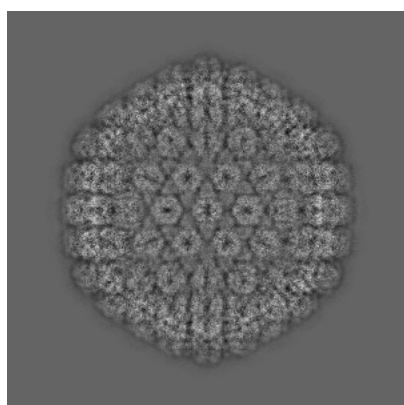
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6907. These allow visual inspection of the internal detail of the map and identification of artifacts.

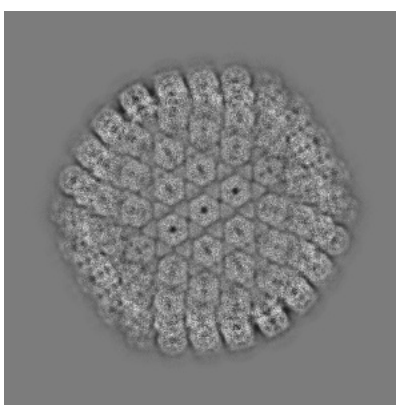
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

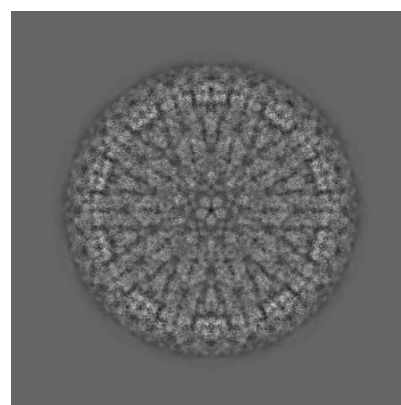
#### 6.1.1 Primary map



X



Y

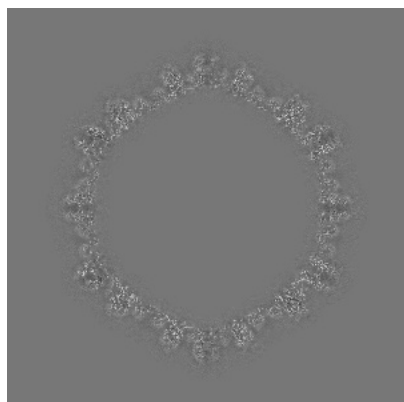


Z

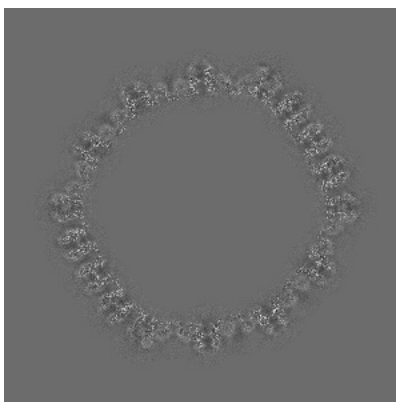
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

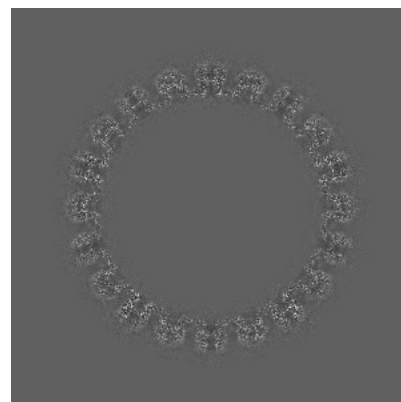
#### 6.2.1 Primary map



X Index: 600



Y Index: 600

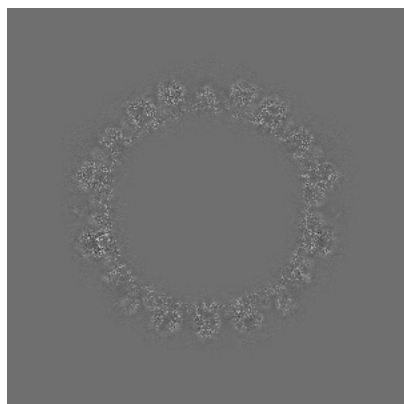


Z Index: 600

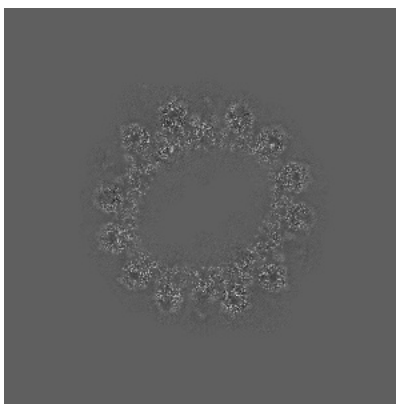
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

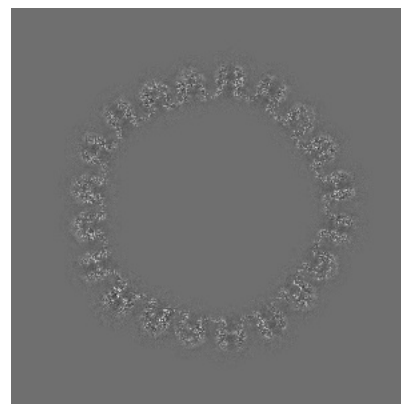
### 6.3.1 Primary map



X Index: 772



Y Index: 319

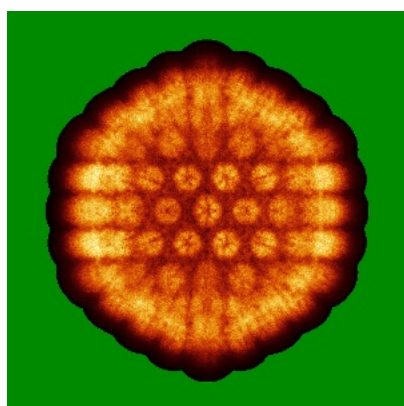


Z Index: 695

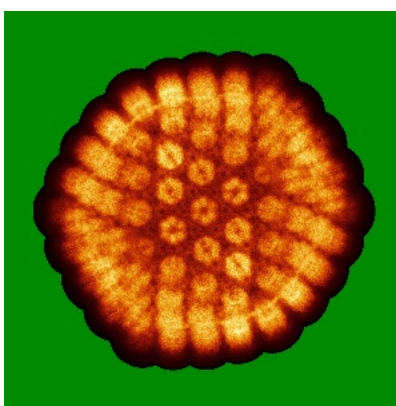
The images above show the largest variance slices of the map in three orthogonal directions.

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

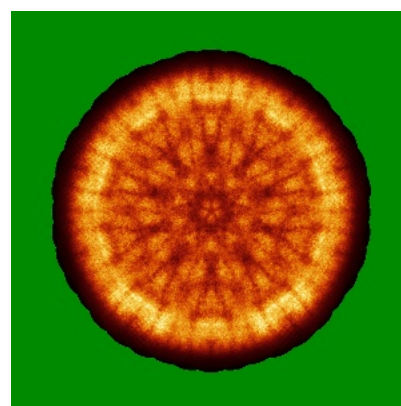
### 6.4.1 Primary map



X



Y

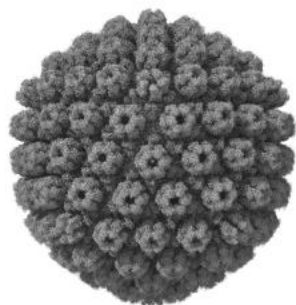


Z

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](#)

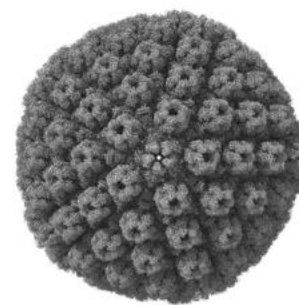
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 12.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

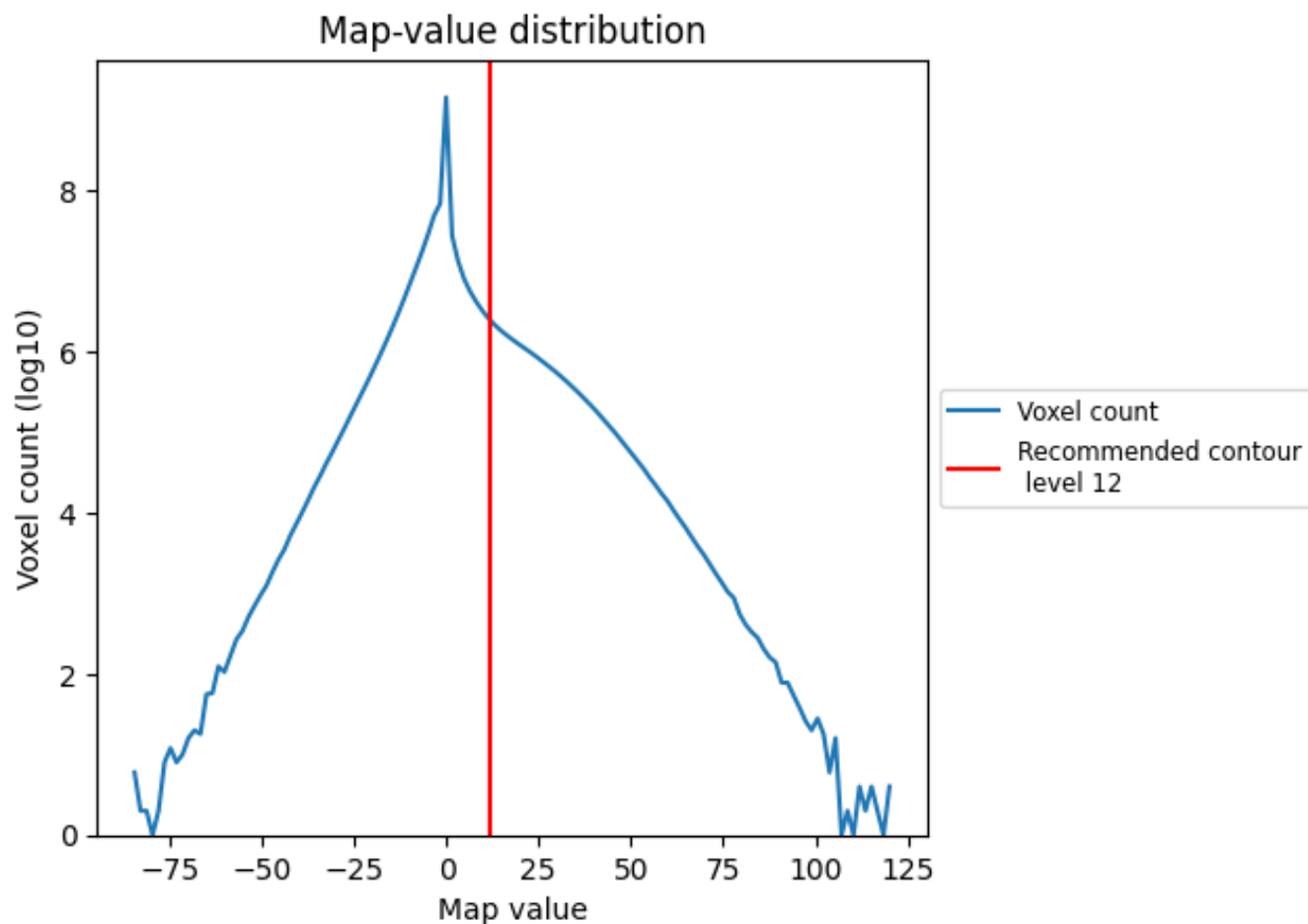
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

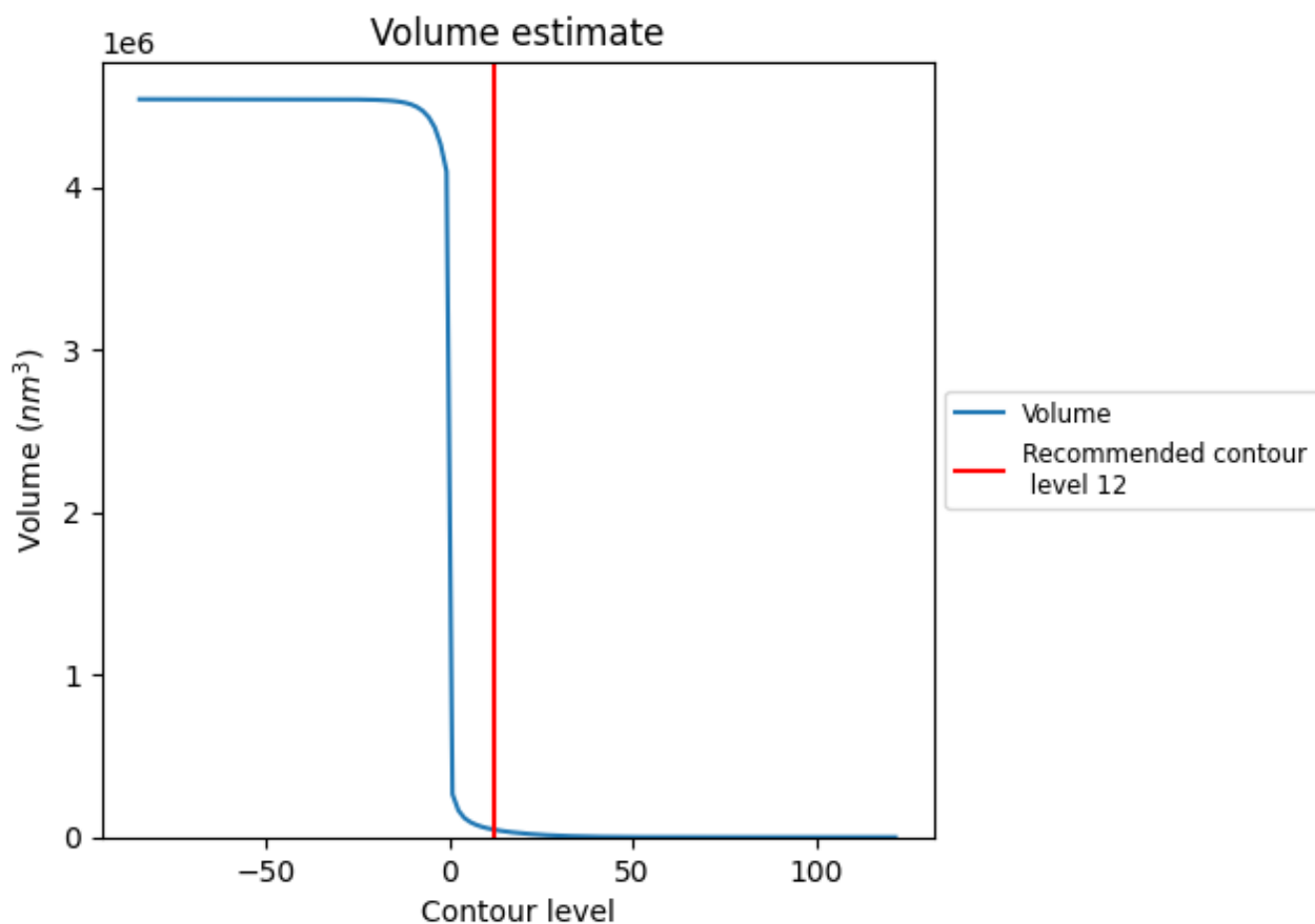
This section contains the results of statistical analysis of the map.

### 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.

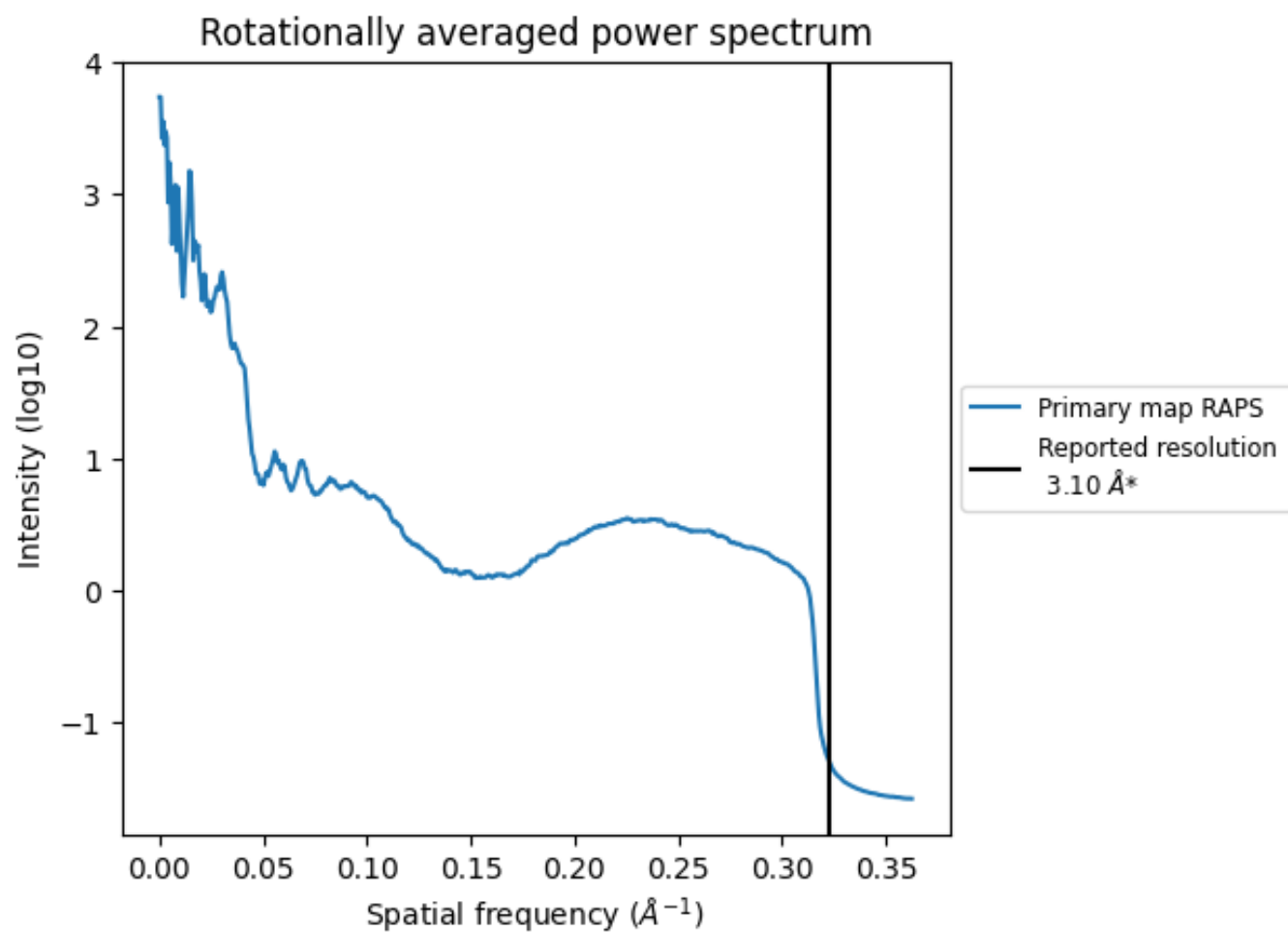
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47511  $\text{nm}^3$ ; this corresponds to an approximate mass of 42918 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 0.323 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

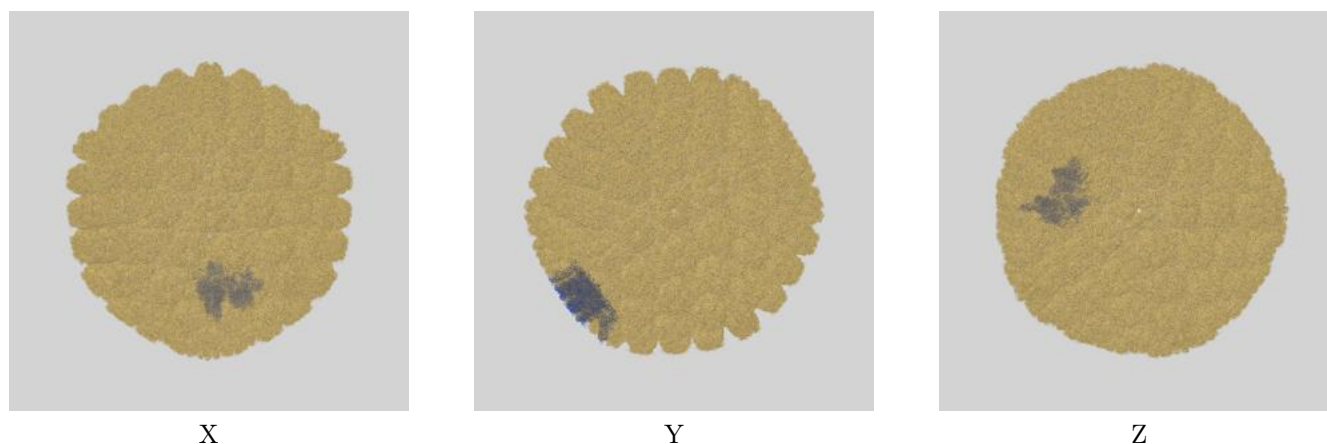
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

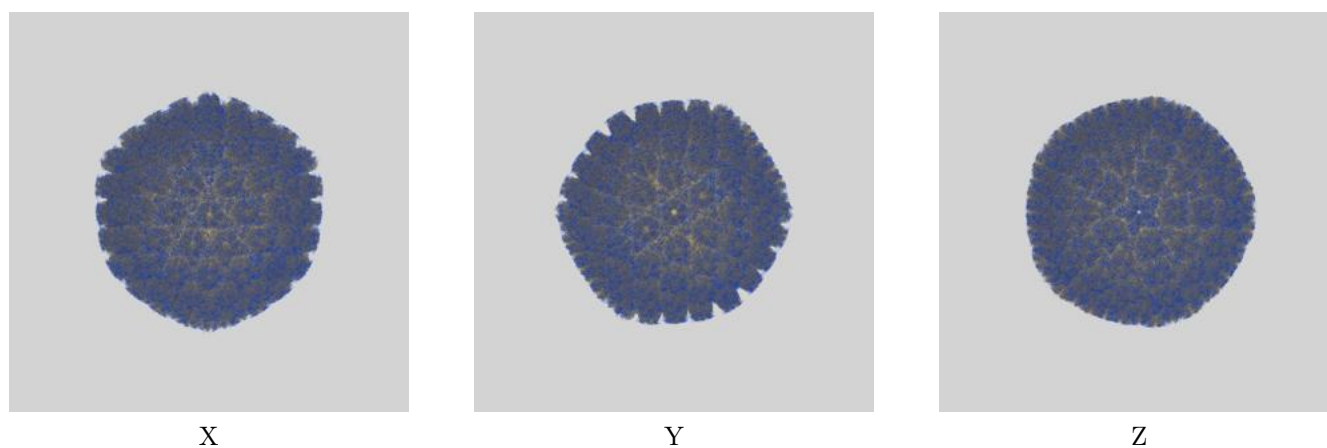
This section contains information regarding the fit between EMDB map EMD-6907 and PDB model 5ZAP. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

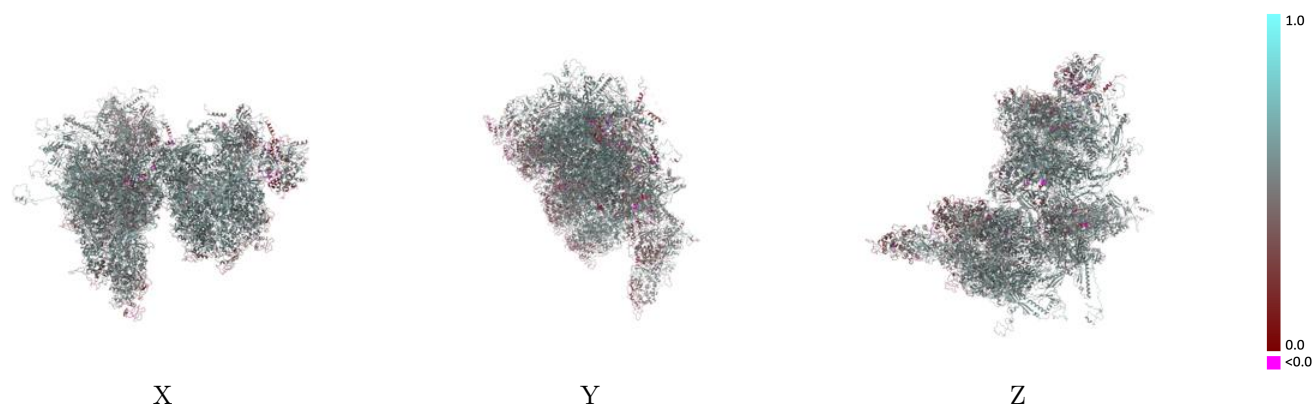


#### 9.1.2 Map-model assembly overlay [i](#)



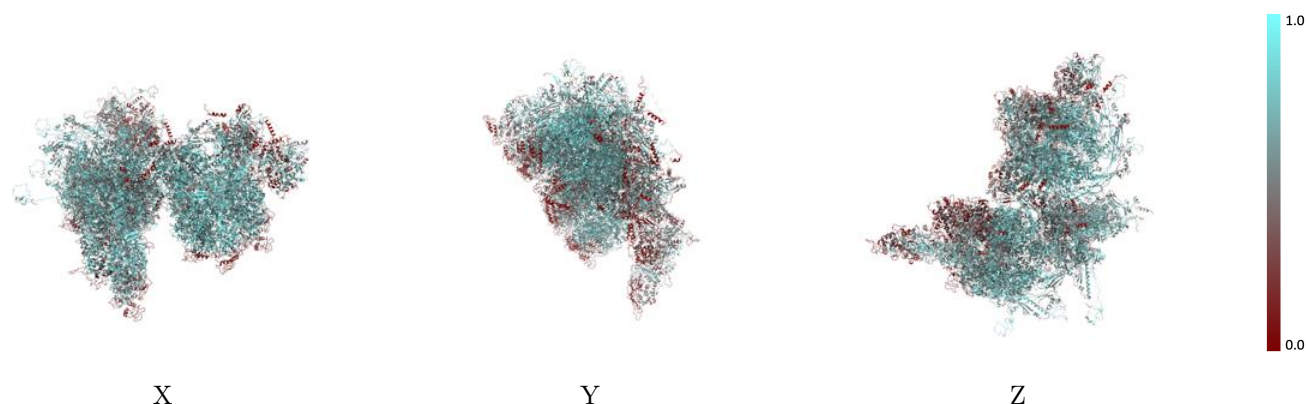
The images above show the 3D surface view of the map at the recommended contour level 12.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



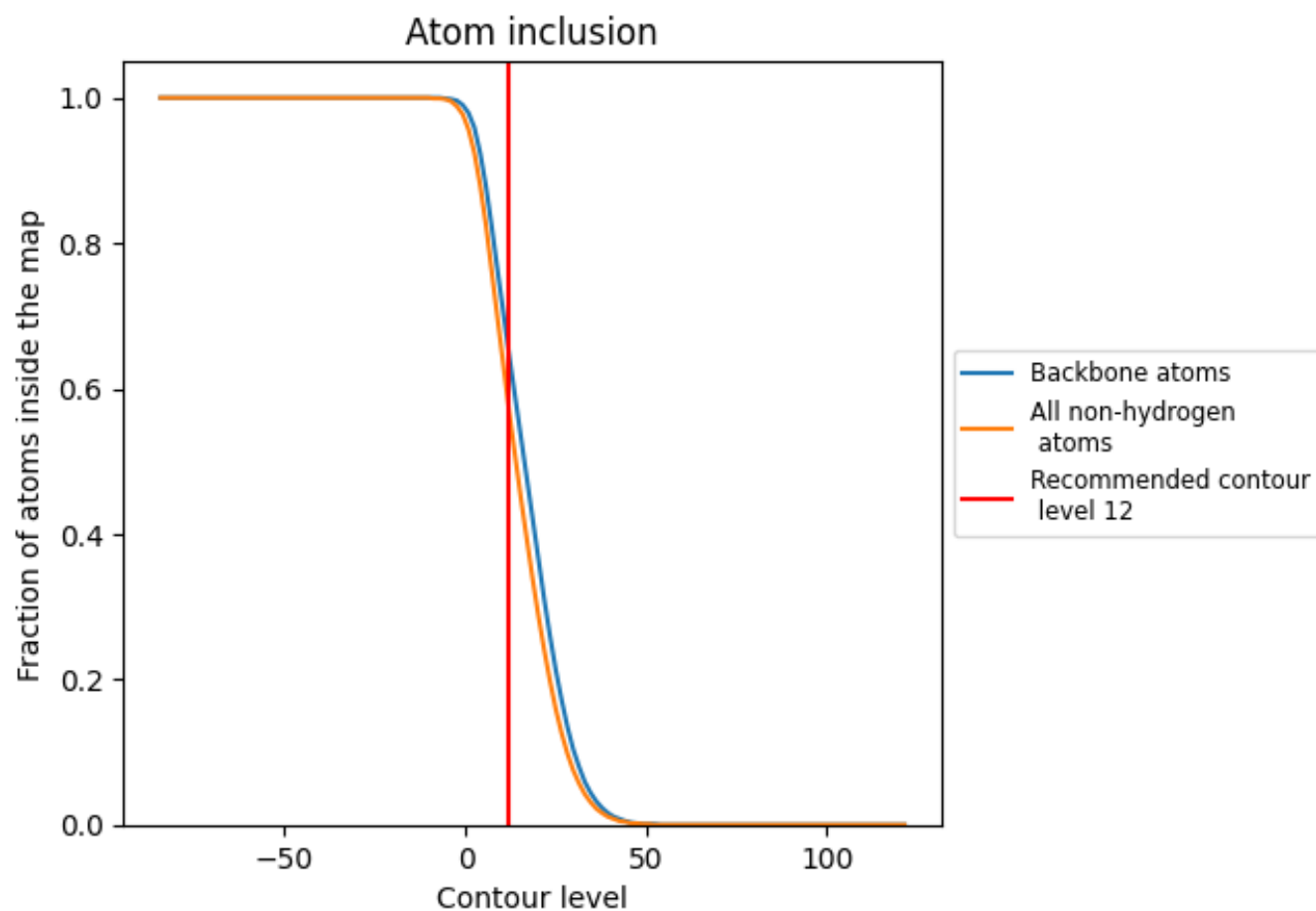
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (12).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 57% 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 (12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5750	 0.4880
A	 0.6240	 0.5110
B	 0.6570	 0.5130
C	 0.6760	 0.5170
D	 0.6200	 0.5140
E	 0.6270	 0.5230
F	 0.6710	 0.5210
G	 0.4050	 0.4200
H	 0.5920	 0.5030
I	 0.6710	 0.5120
J	 0.6030	 0.4880
K	 0.7230	 0.5420
L	 0.7220	 0.5370
M	 0.6800	 0.5410
N	 0.6620	 0.5310
O	 0.6860	 0.5300
P	 0.6920	 0.5270
Q	 0.2850	 0.3950
R	 0.2600	 0.3700
S	 0.1760	 0.3810
T	 0.4530	 0.4700
U	 0.4800	 0.4750
V	 0.2670	 0.3970
W	 0.4530	 0.4400
X	 0.4640	 0.4480
Y	 0.2970	 0.3920
Z	 0.4640	 0.4230
a	 0.4170	 0.3570
b	 0.2870	 0.3550
c	 0.4750	 0.4860
d	 0.5110	 0.4820
e	 0.2820	 0.4150
f	 0.1530	 0.3980
g	 0.0750	 0.2750
h	 0.0690	 0.2780



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.1050	 0.2800
j	 0.0640	 0.3190
k	 0.1040	 0.2930
l	 0.1210	 0.2810
m	 0.0460	 0.2520
n	 0.1040	 0.2720
o	 0.0580	 0.1720
p	 0.1280	 0.2930
q	 0.1180	 0.3040
r	 0.0980	 0.2730
s	 0.0890	 0.2860
t	 0.0860	 0.2950