



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 12:58 AM EDT

PDB ID : 6NHJ
EMDB ID : EMD-9366
Title : Atomic structures and deletion mutant reveal different capsid-binding patterns and functional significance of tegument protein pp150 in murine and human cytomegaloviruses with implications for therapeutic development
Authors : Liu, W.; Dai, X.H.; Jih, J.; Chan, K.; Trang, P.; Yu, X.K.; Balogun, R.; Mei, Y.; Liu, F.Y.; Zhou, Z.H.
Deposited on : 2018-12-22
Resolution : 5.00 Å(reported)

This is a Full wwPDB EM Validation 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:

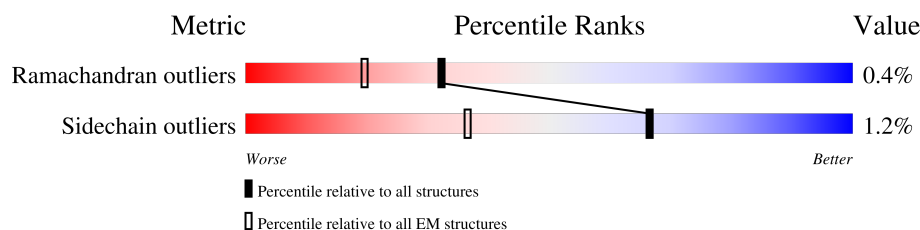
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.00 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 $\leq 5\%$. 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	1353	<div> <div>28%</div> <div>98%</div> <div>..</div> </div>
1	B	1353	<div> <div>27%</div> <div>96%</div> <div>..</div> </div>
1	C	1353	<div> <div>30%</div> <div>95%</div> <div>..</div> </div>
1	D	1353	<div> <div>30%</div> <div>96%</div> <div>..</div> </div>
1	E	1353	<div> <div>28%</div> <div>98%</div> <div>..</div> </div>
1	F	1353	<div> <div>28%</div> <div>96%</div> <div>..</div> </div>
1	G	1353	<div> <div>32%</div> <div>98%</div> <div>..</div> </div>
1	H	1353	<div> <div>34%</div> <div>98%</div> <div>..</div> </div>
1	I	1353	<div> <div>33%</div> <div>97%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	k	1353	36% 94% ..
1	l	1353	30% 97% ..
1	m	1353	31% 95% ..
1	n	1353	35% 98% ..
1	o	1353	31% 96% ..
1	p	1353	33% 95% ..
1	q	1353	54% 89% 10%
2	2	718	24% 23% 76%
2	3	718	28% 27% 72%
2	e	718	11% 23% 76%
2	f	718	14% 23% 76%
2	g	718	14% 23% 76%
2	h	718	13% 27% 72%
2	i	718	14% 27% 72%
2	j	718	15% 27% 72%
3	J	98	22% 60% 39%
3	K	98	30% 60% 40%
3	L	98	27% 60% 40%
3	M	98	32% 60% 40%
3	N	98	27% 59% 40%
3	O	98	29% 60% 40%
3	P	98	26% 59% 40%
3	Q	98	29% 60% 40%
3	R	98	29% 60% 40%
3	r	98	27% 59% 39%

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Mol	Chain	Length	Quality of chain
3	s	98	
3	t	98	
3	u	98	
3	v	98	
3	w	98	
3	x	98	
4	S	294	
4	T	294	
4	U	294	
4	V	294	
4	y	294	
5	1	311	
5	W	311	
5	X	311	
5	Y	311	
5	Z	311	
5	a	311	
5	b	311	
5	c	311	
5	d	311	
5	z	311	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 218639 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	1335	Total	C	N	O	S	0	0
			10537	6666	1856	1962	53		
1	B	1310	Total	C	N	O	S	0	0
			10351	6550	1822	1926	53		
1	C	1310	Total	C	N	O	S	0	0
			10350	6551	1822	1924	53		
1	D	1314	Total	C	N	O	S	0	0
			10375	6567	1826	1929	53		
1	E	1330	Total	C	N	O	S	0	0
			10495	6635	1852	1955	53		
1	F	1319	Total	C	N	O	S	0	0
			10407	6585	1831	1938	53		
1	G	1341	Total	C	N	O	S	0	0
			10580	6692	1864	1971	53		
1	H	1341	Total	C	N	O	S	0	0
			10580	6692	1864	1971	53		
1	I	1321	Total	C	N	O	S	0	0
			10421	6593	1834	1941	53		
1	k	1295	Total	C	N	O	S	0	0
			10209	6465	1795	1896	53		
1	l	1336	Total	C	N	O	S	0	0
			10548	6673	1859	1963	53		
1	m	1312	Total	C	N	O	S	0	0
			10364	6559	1824	1928	53		
1	n	1335	Total	C	N	O	S	0	0
			10538	6663	1858	1964	53		
1	o	1313	Total	C	N	O	S	0	0
			10368	6558	1828	1929	53		
1	p	1301	Total	C	N	O	S	0	0
			10252	6477	1813	1910	52		
1	q	1219	Total	C	N	O	S	0	0
			9621	6090	1690	1791	50		

- Molecule 2 is a protein called Tegument protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	174	Total 1469	C 929	N 279	O 255	S 6	0	0
2	3	200	Total 1665	C 1052	N 314	O 291	S 8	0	0
2	e	174	Total 1469	C 929	N 279	O 255	S 6	0	0
2	h	200	Total 1665	C 1052	N 314	O 291	S 8	0	0
2	f	174	Total 1469	C 929	N 279	O 255	S 6	0	0
2	i	200	Total 1665	C 1052	N 314	O 291	S 8	0	0
2	g	174	Total 1469	C 929	N 279	O 255	S 6	0	0
2	j	200	Total 1665	C 1052	N 314	O 291	S 8	0	0

- Molecule 3 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	60	Total 471	C 300	N 83	O 83	S 5	0	0
3	K	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	L	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	M	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	N	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	O	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	P	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	Q	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	R	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	r	60	Total 471	C 300	N 83	O 83	S 5	0	0
3	s	59	Total 462	C 294	N 81	O 82	S 5	0	0
3	t	59	Total 462	C 294	N 81	O 82	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	u	60	Total	C	N	O	S	0	0
			471	300	83	83	5		
3	v	60	Total	C	N	O	S	0	0
			471	300	83	83	5		
3	w	60	Total	C	N	O	S	0	0
			471	300	83	83	5		
3	x	57	Total	C	N	O	S	0	0
			450	287	79	79	5		

- Molecule 4 is a protein called Minor capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	y	249	Total	C	N	O	S	0	0
			1977	1261	350	356	10		
4	S	289	Total	C	N	O	S	0	0
			2305	1470	406	416	13		
4	T	289	Total	C	N	O	S	0	0
			2305	1470	406	416	13		
4	U	289	Total	C	N	O	S	0	0
			2305	1470	406	416	13		
4	V	289	Total	C	N	O	S	0	0
			2305	1470	406	416	13		

- Molecule 5 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	z	284	Total	C	N	O	S	0	0
			2224	1403	382	419	20		
5	W	281	Total	C	N	O	S	0	0
			2201	1390	378	414	19		
5	X	277	Total	C	N	O	S	0	0
			2166	1367	373	407	19		
5	Y	282	Total	C	N	O	S	0	0
			2209	1395	379	415	20		
5	Z	281	Total	C	N	O	S	0	0
			2201	1390	378	414	19		
5	1	257	Total	C	N	O	S	0	0
			2009	1268	350	374	17		
5	a	267	Total	C	N	O	S	0	0
			2085	1314	363	389	19		
5	b	270	Total	C	N	O	S	0	0
			2109	1330	366	394	19		

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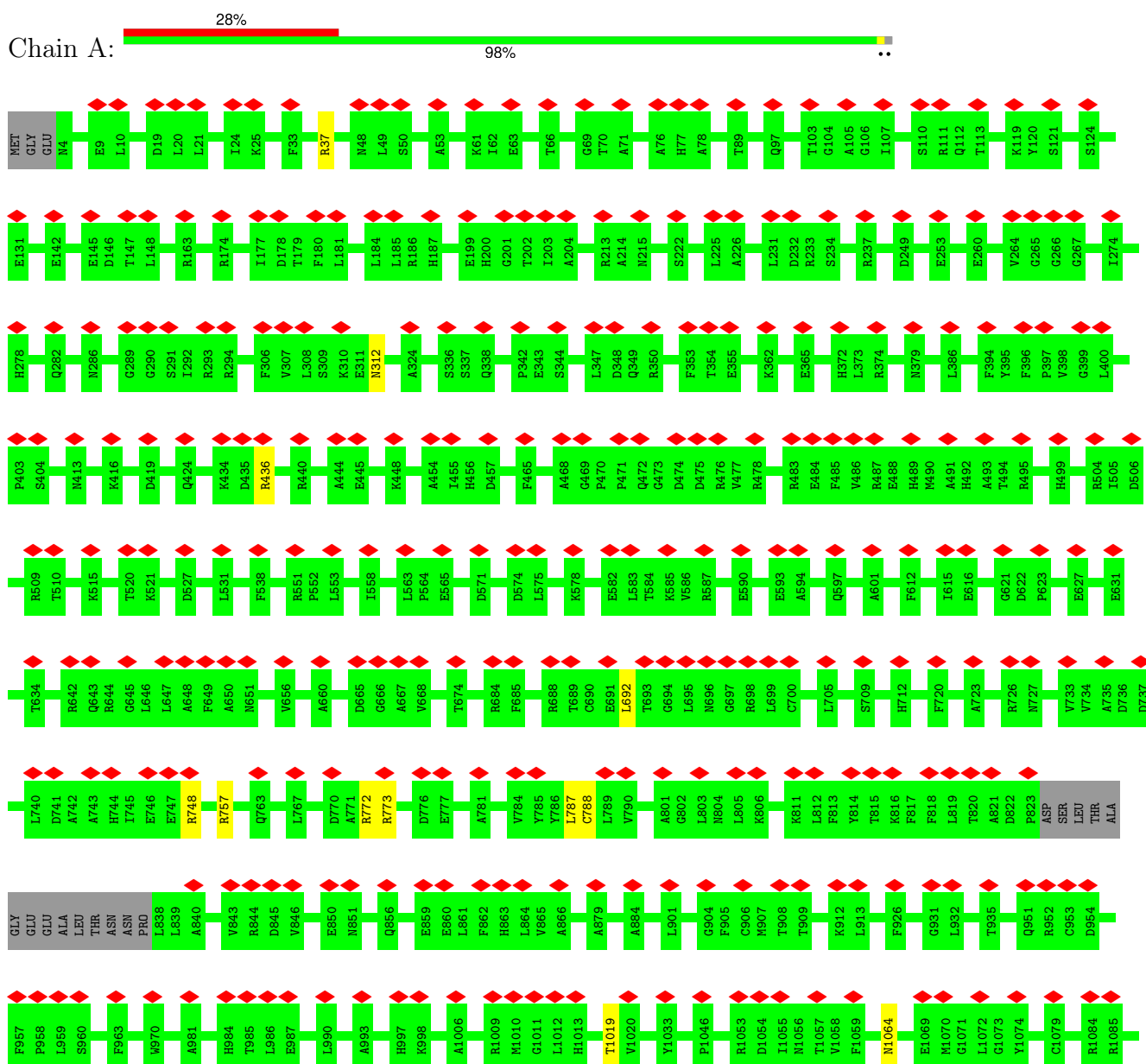
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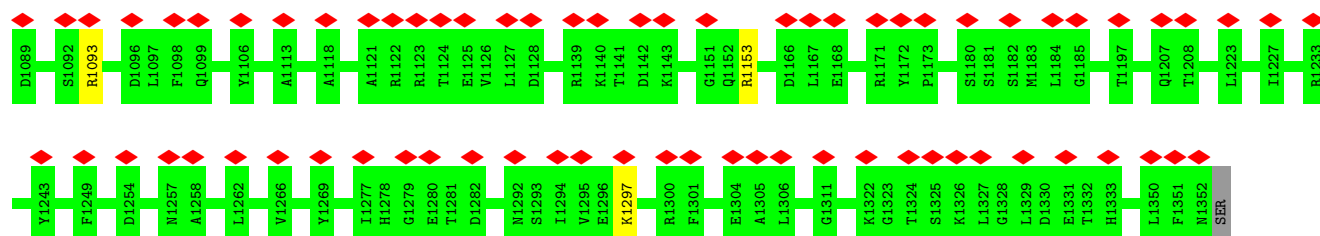
Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	274	Total	C	N	O	S	0	0
			2141	1349	371	401	20		
5	d	274	Total	C	N	O	S	0	0
			2140	1351	370	399	20		

3 Residue-property plots

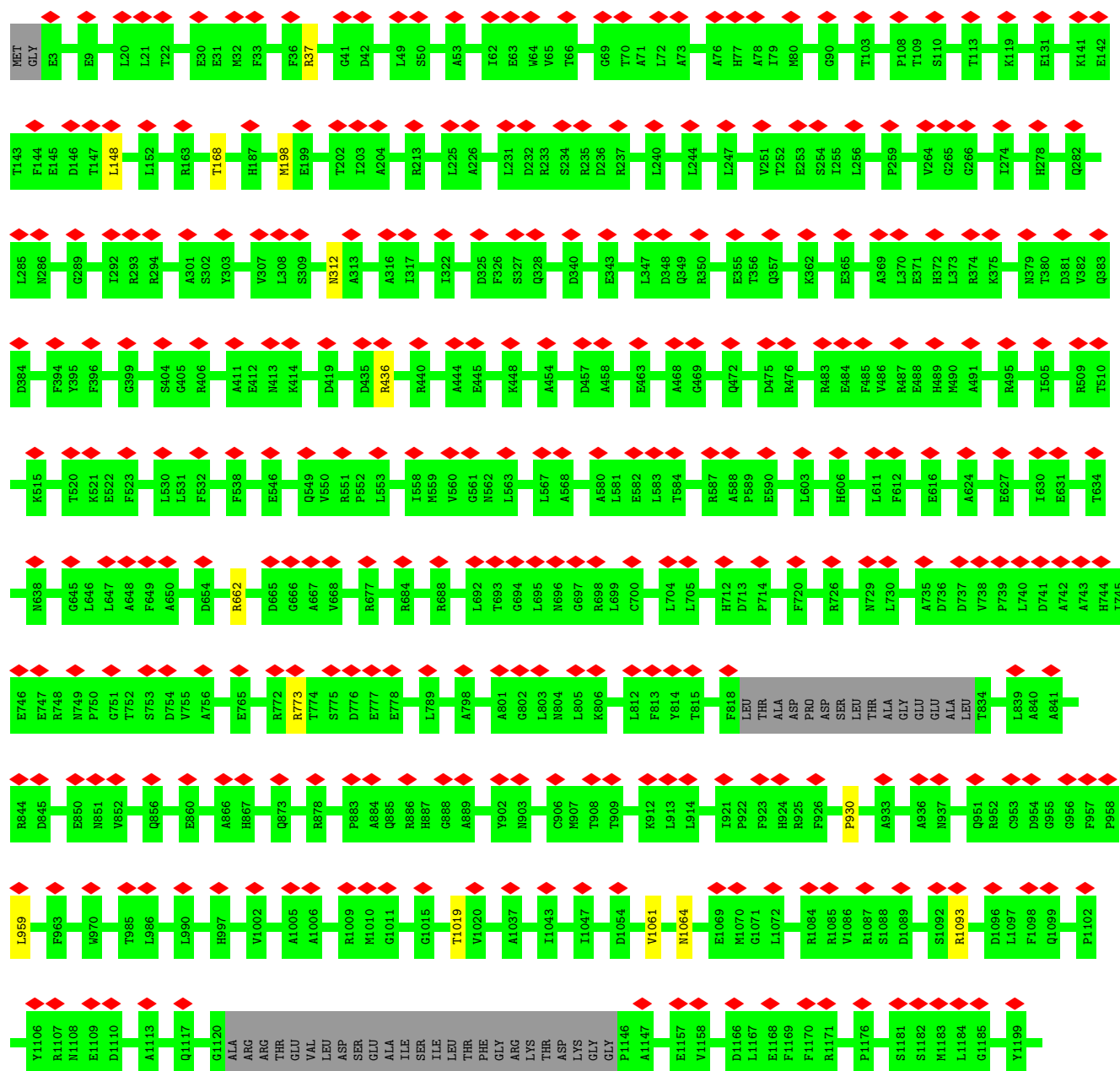
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

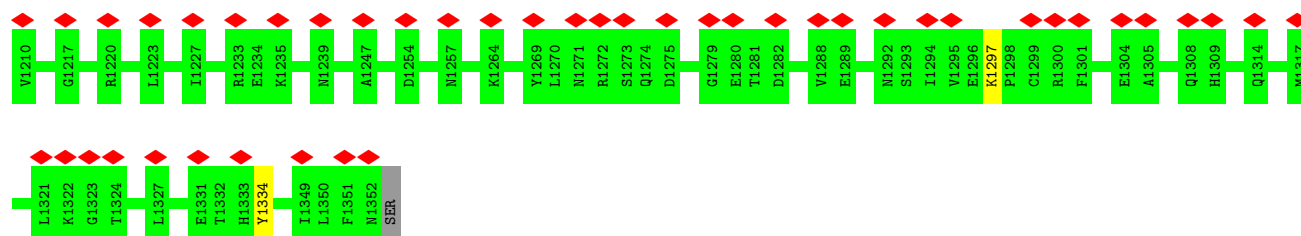
- Molecule 1: Major capsid protein





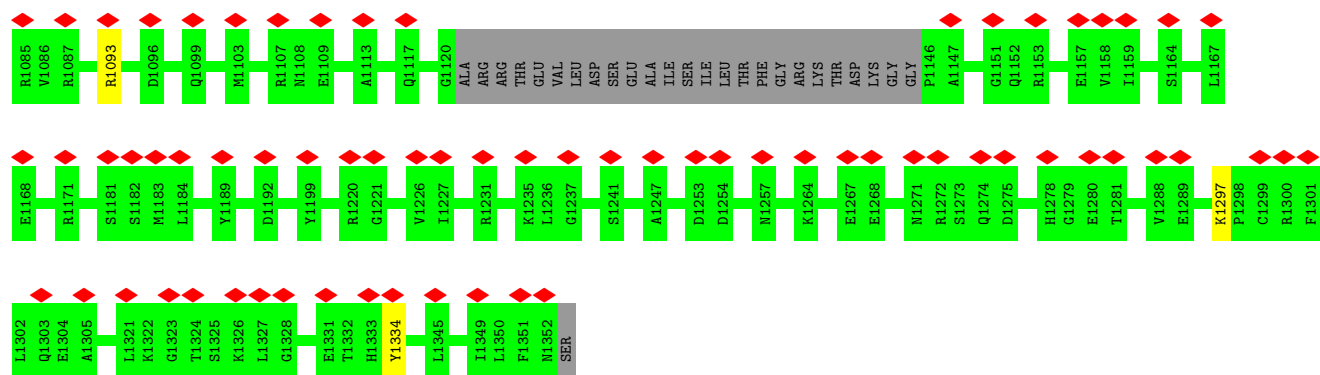
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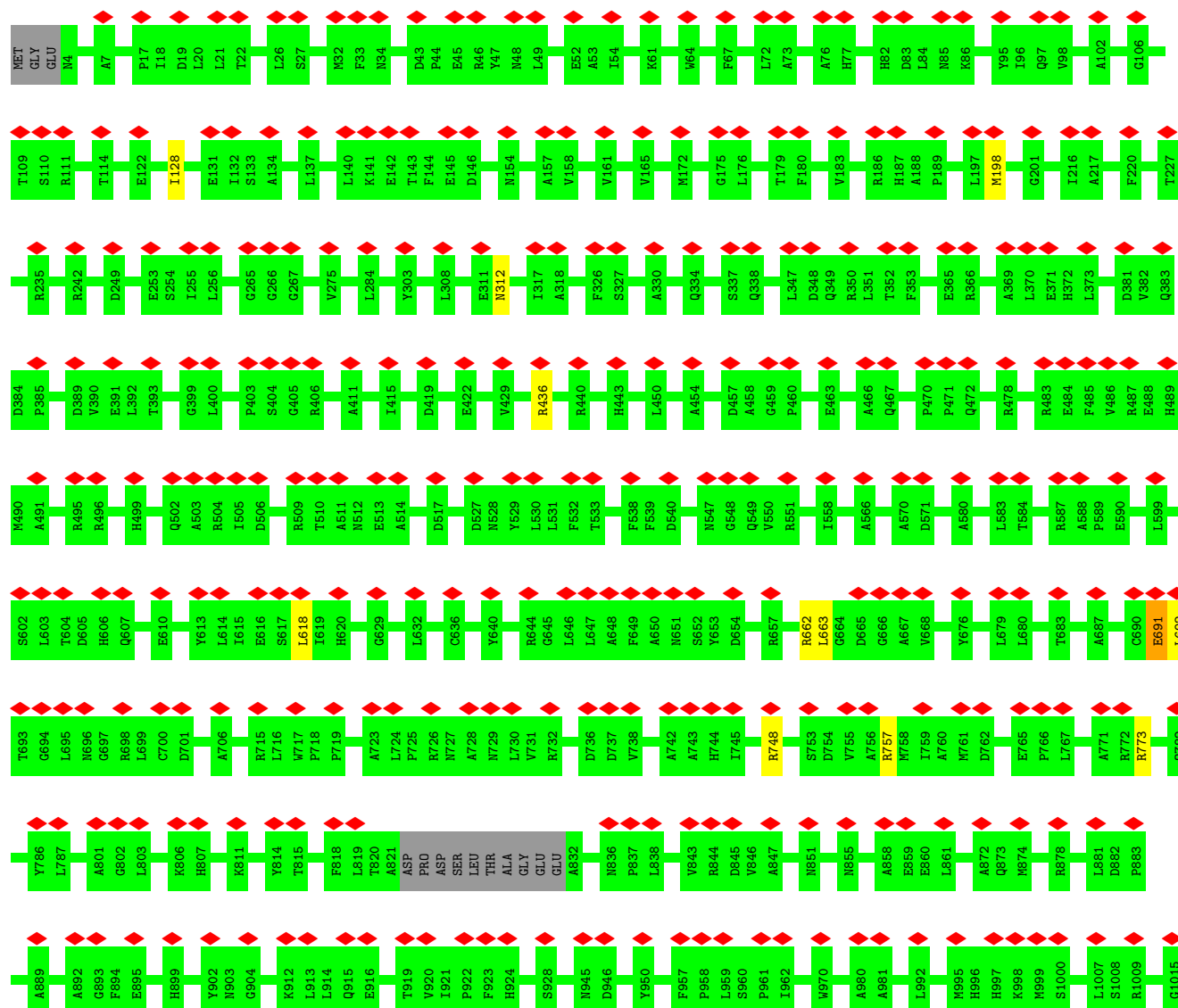


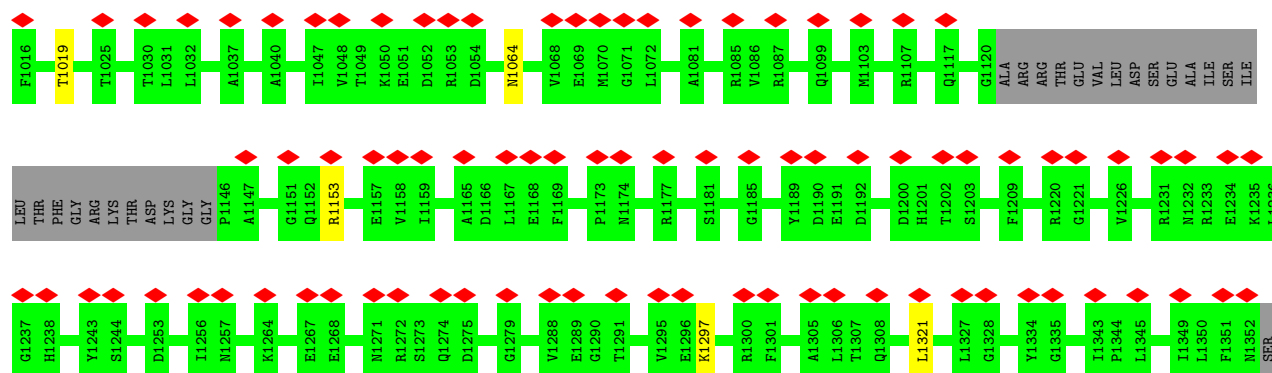
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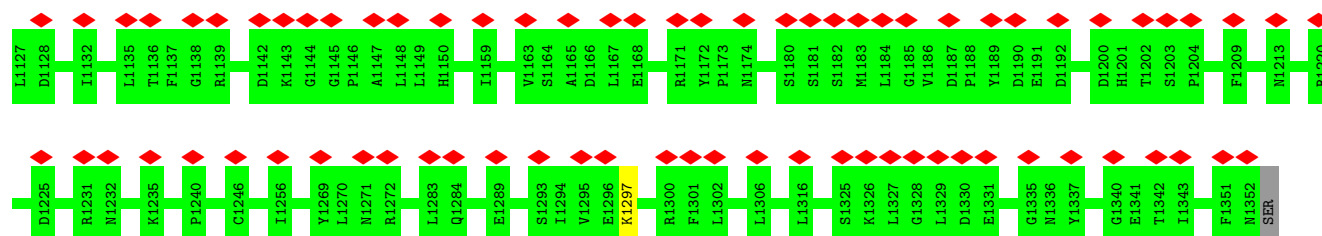
• Molecule 1: Major capsid protein



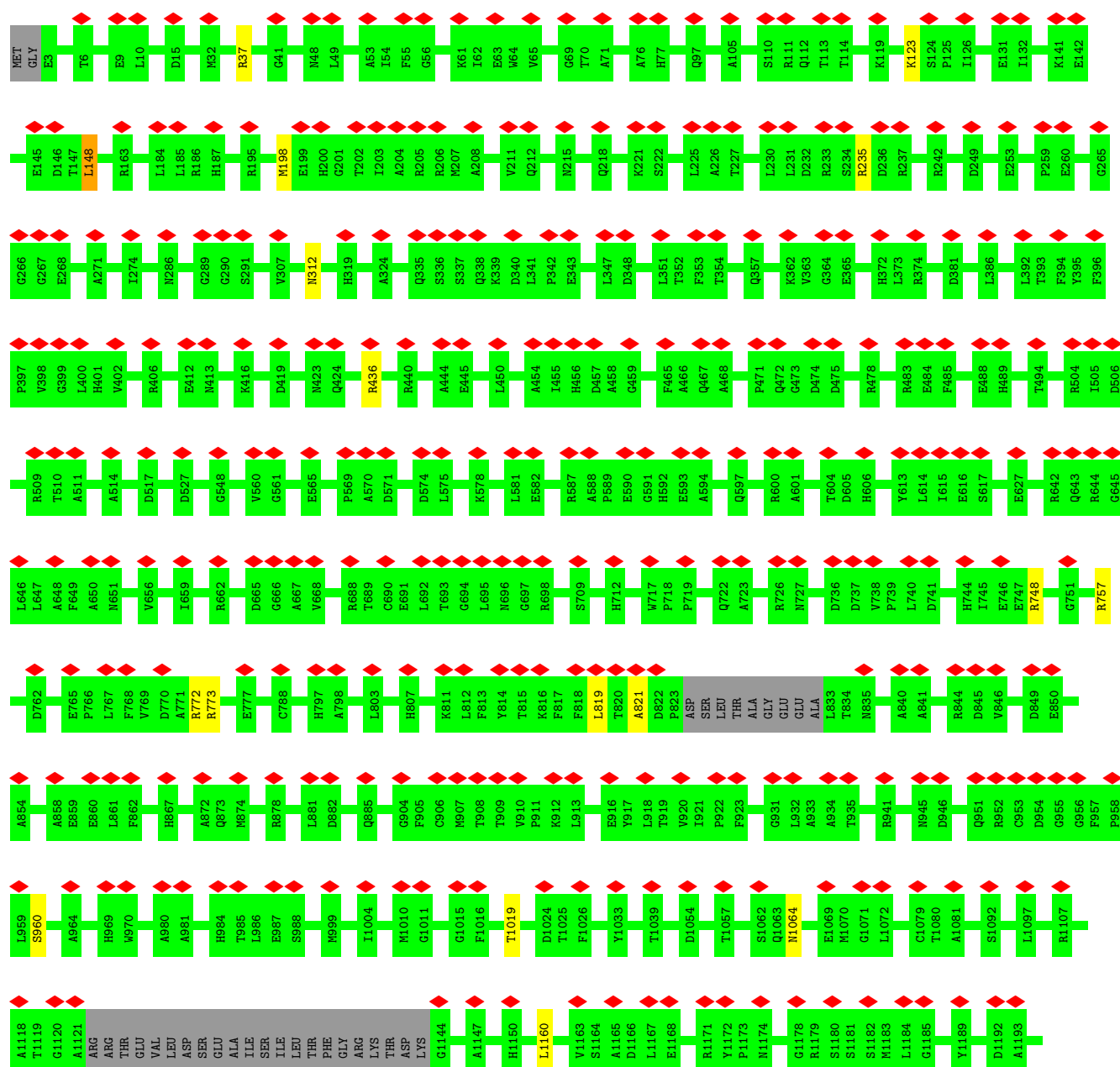


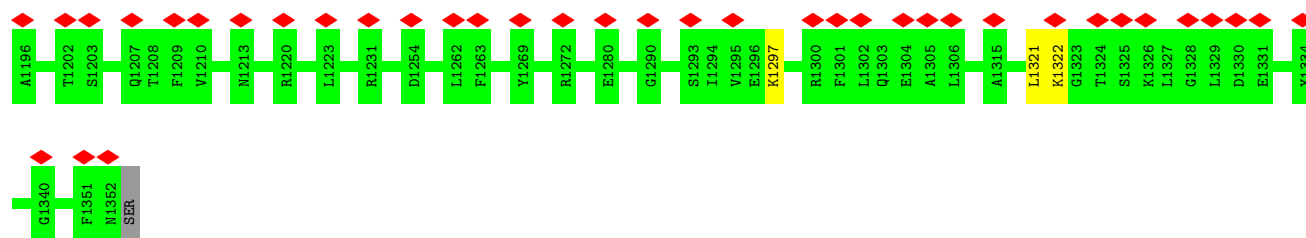
• Molecule 1: Major capsid protein



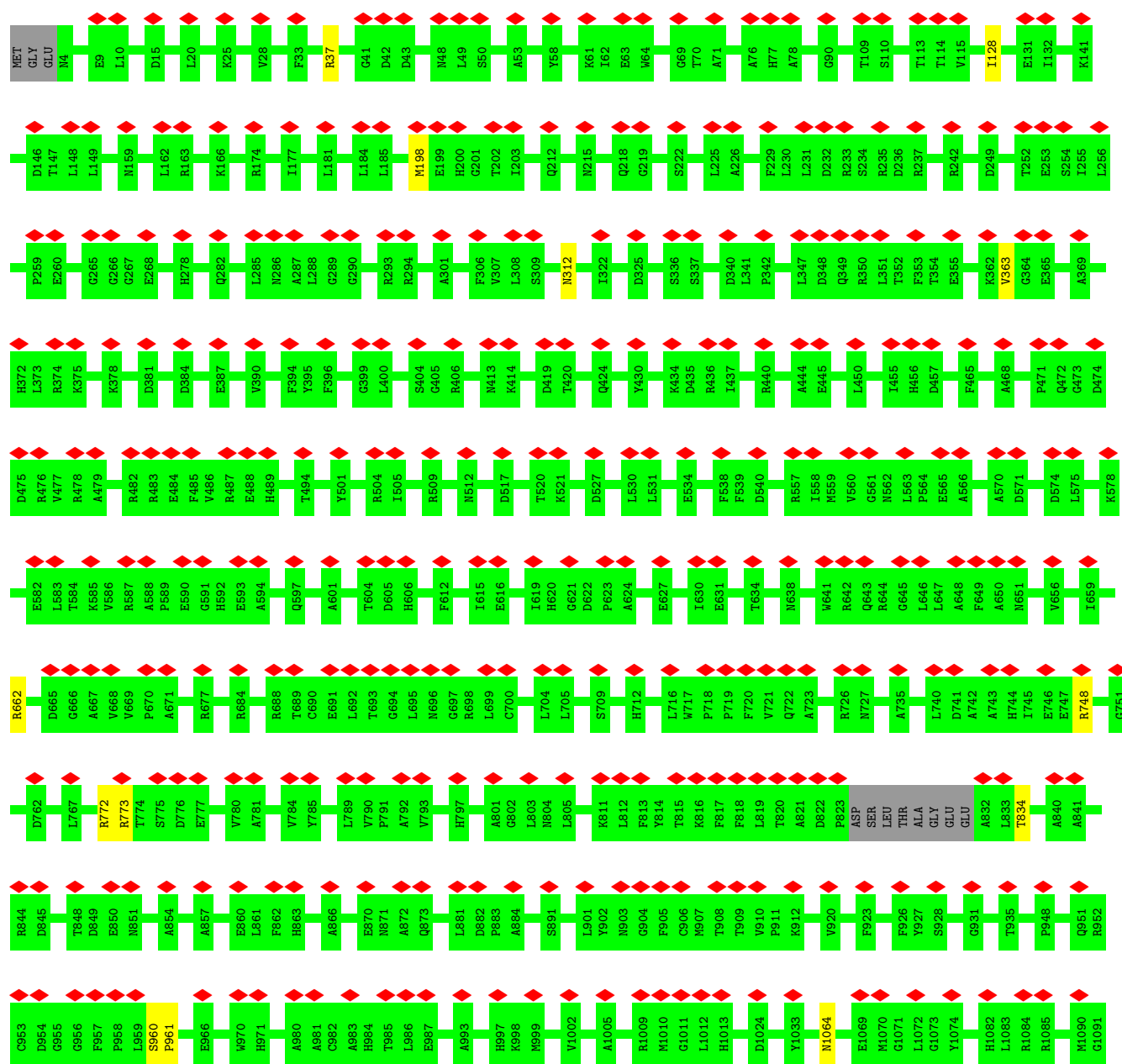


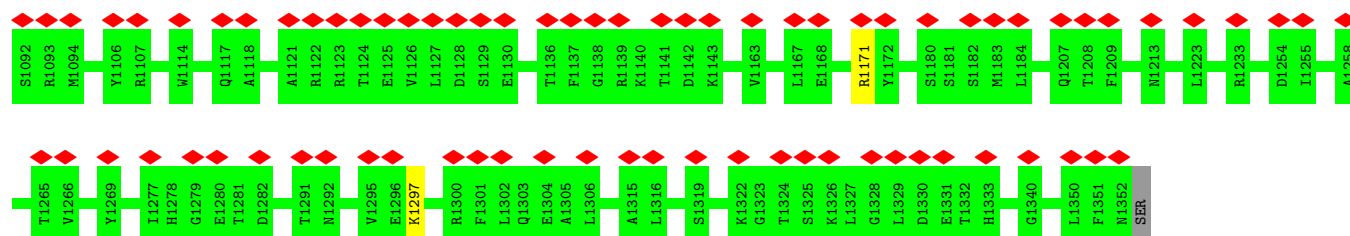
• Molecule 1: Major capsid protein





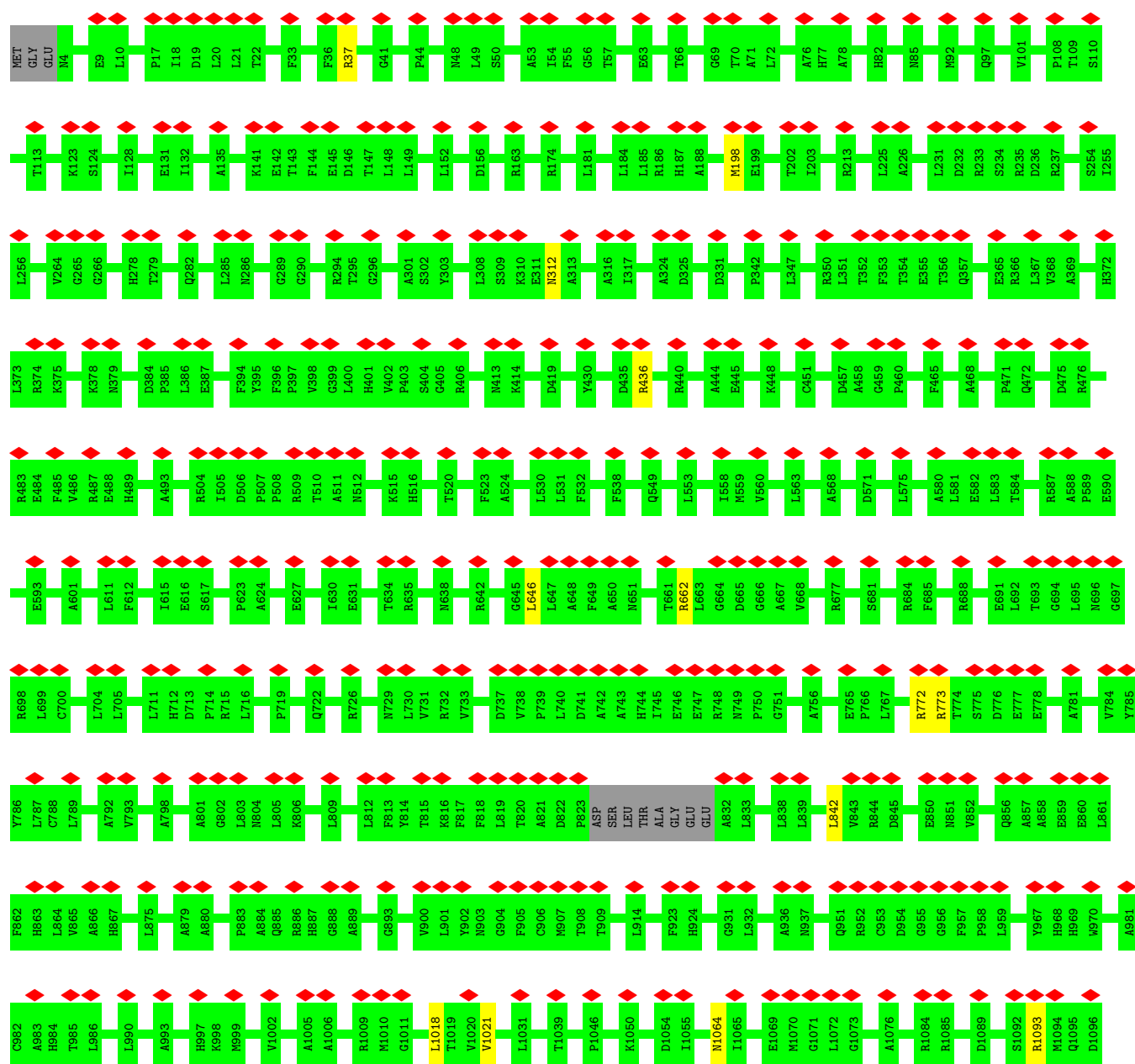
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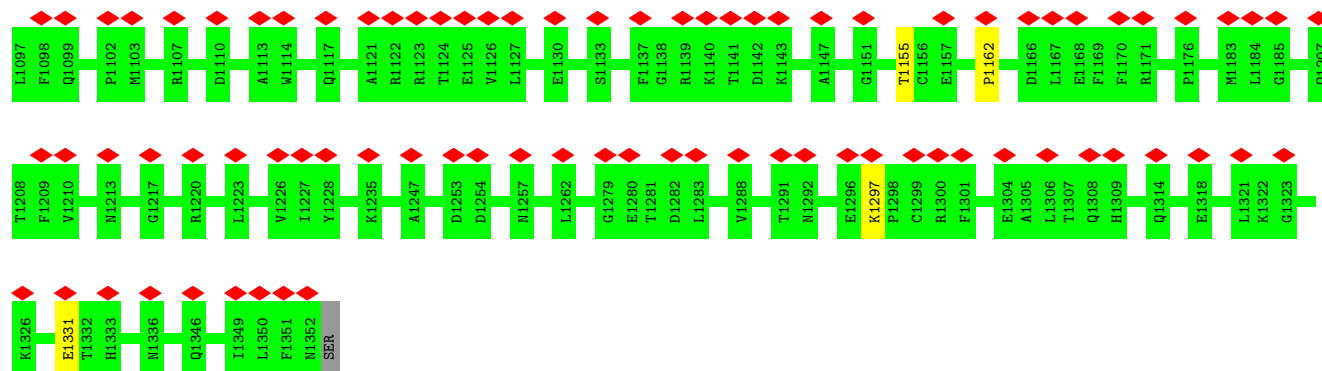




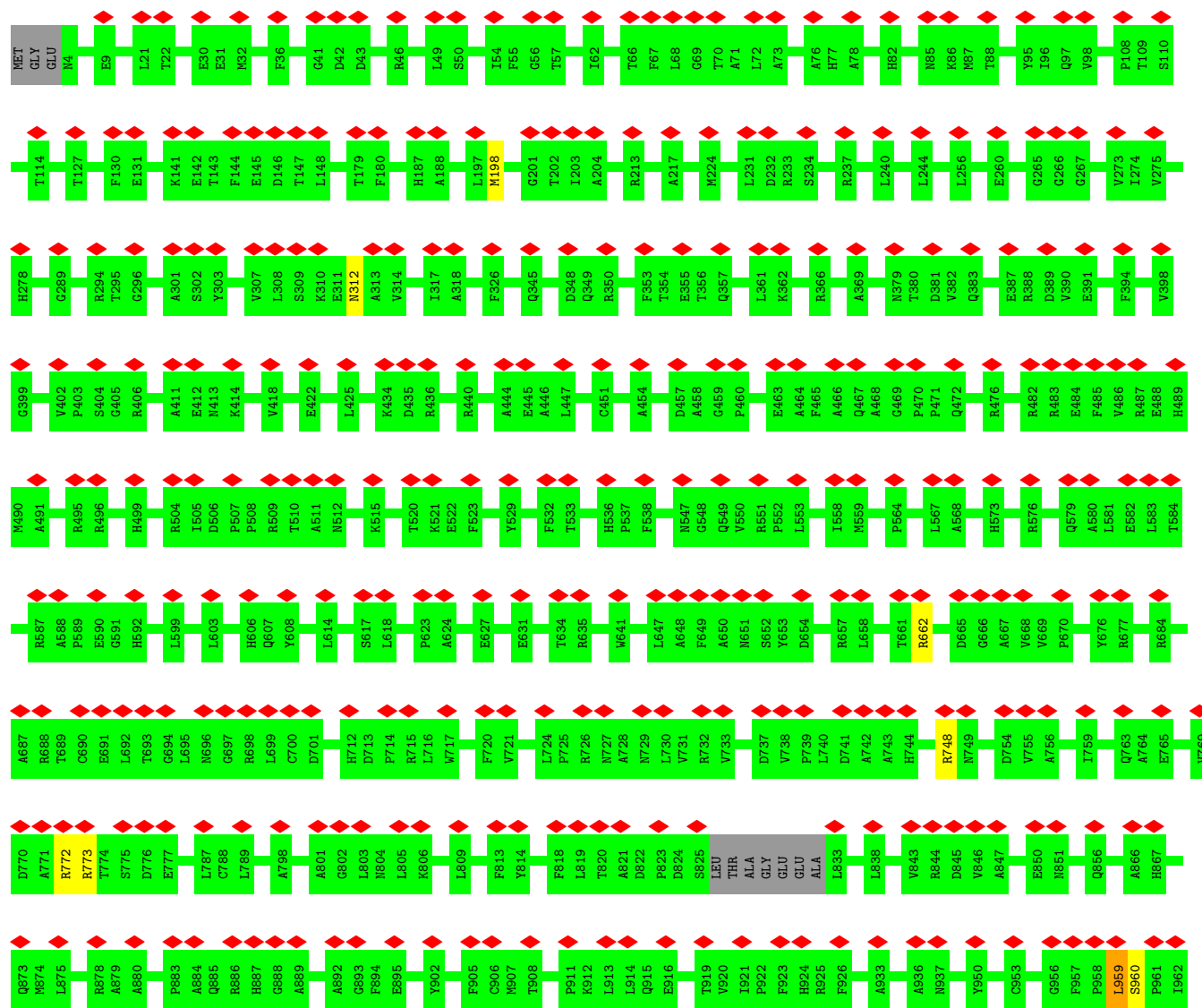
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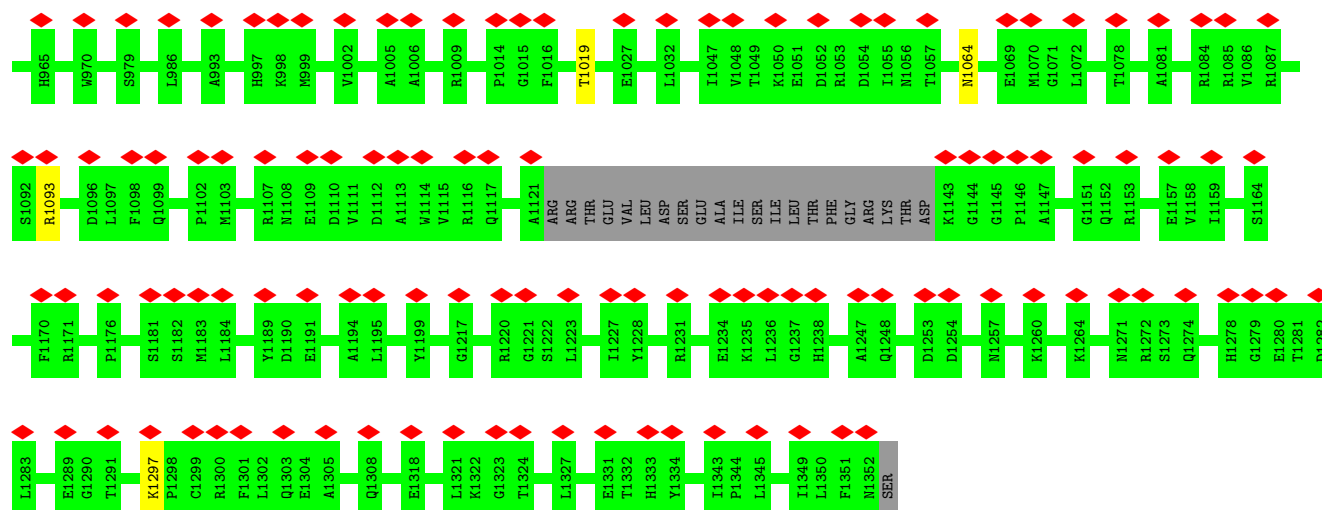
Chain H: 34% 98%



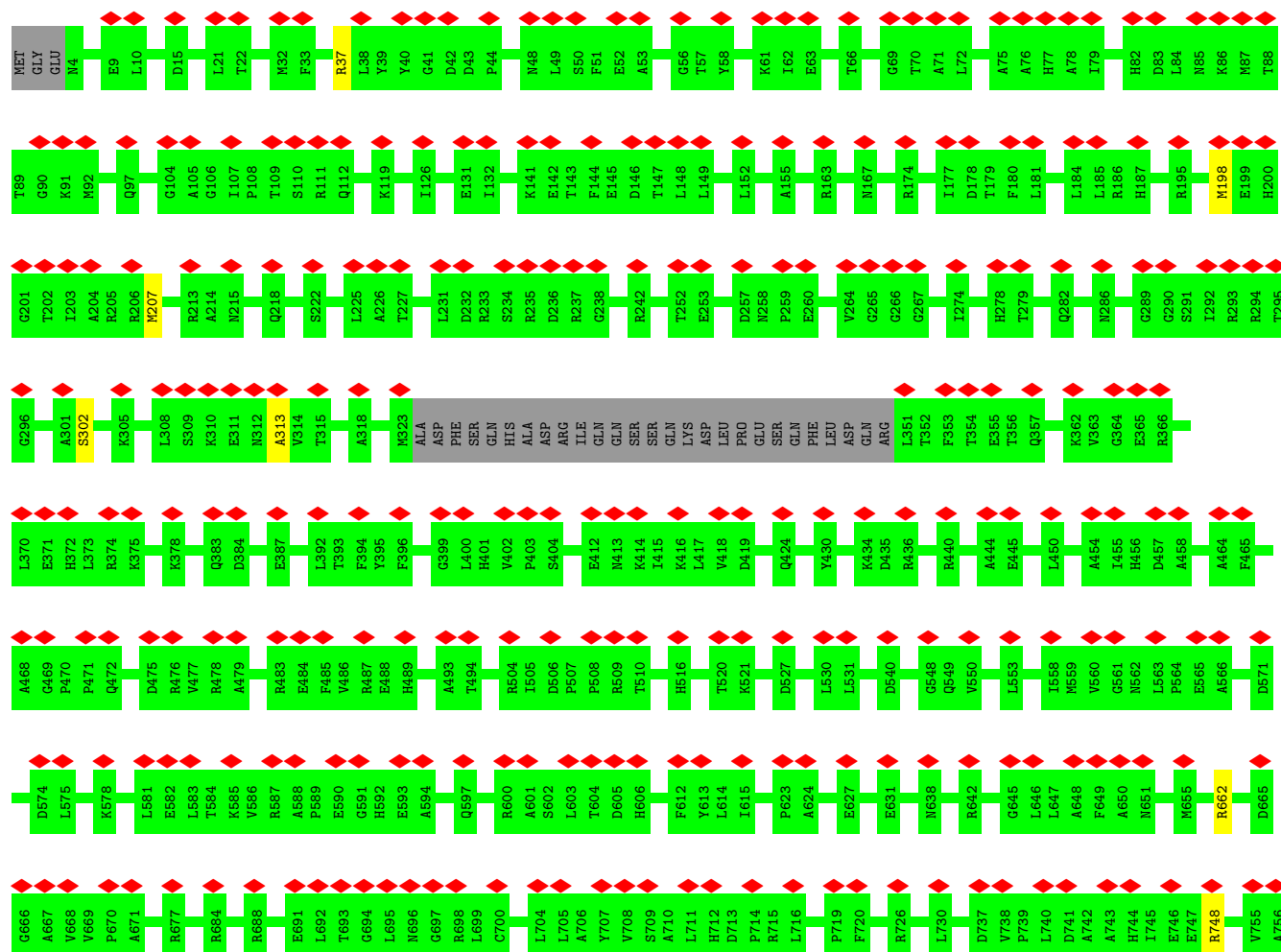


• Molecule 1: Major capsid protein



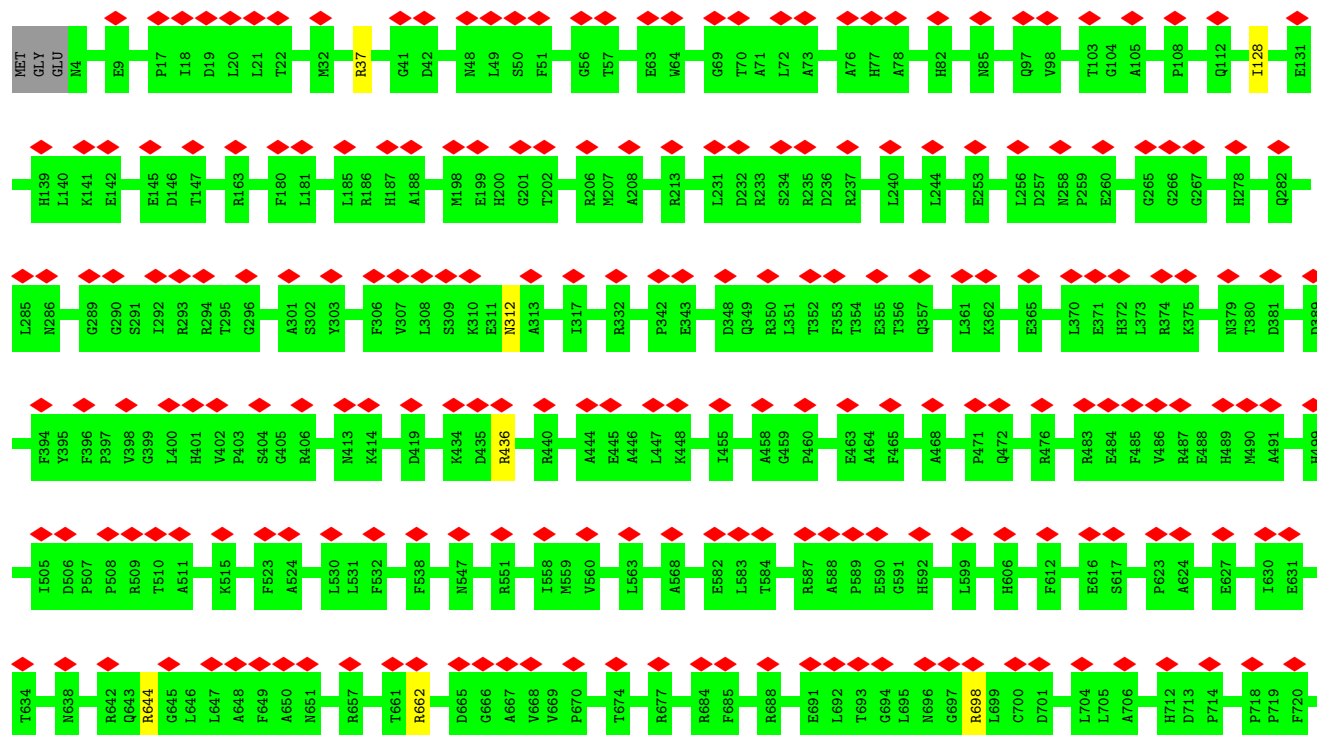


• Molecule 1: Major capsid protein



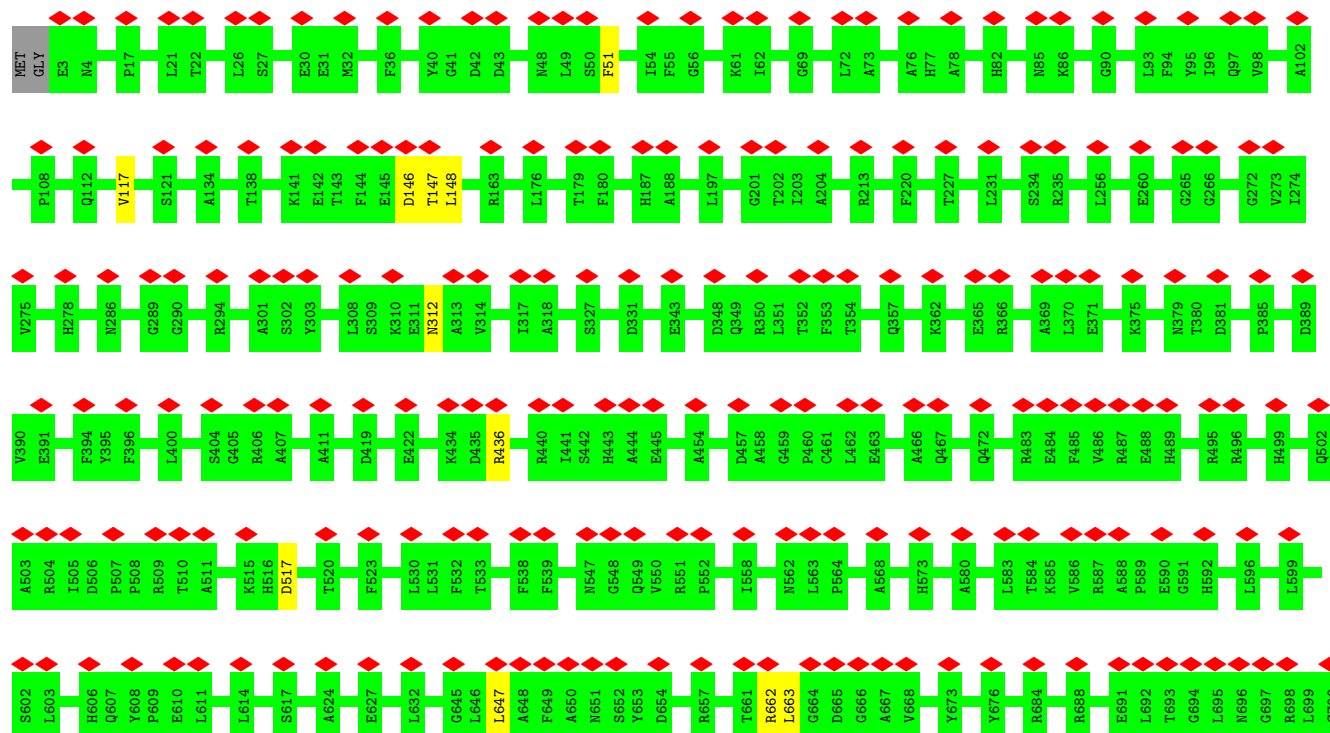


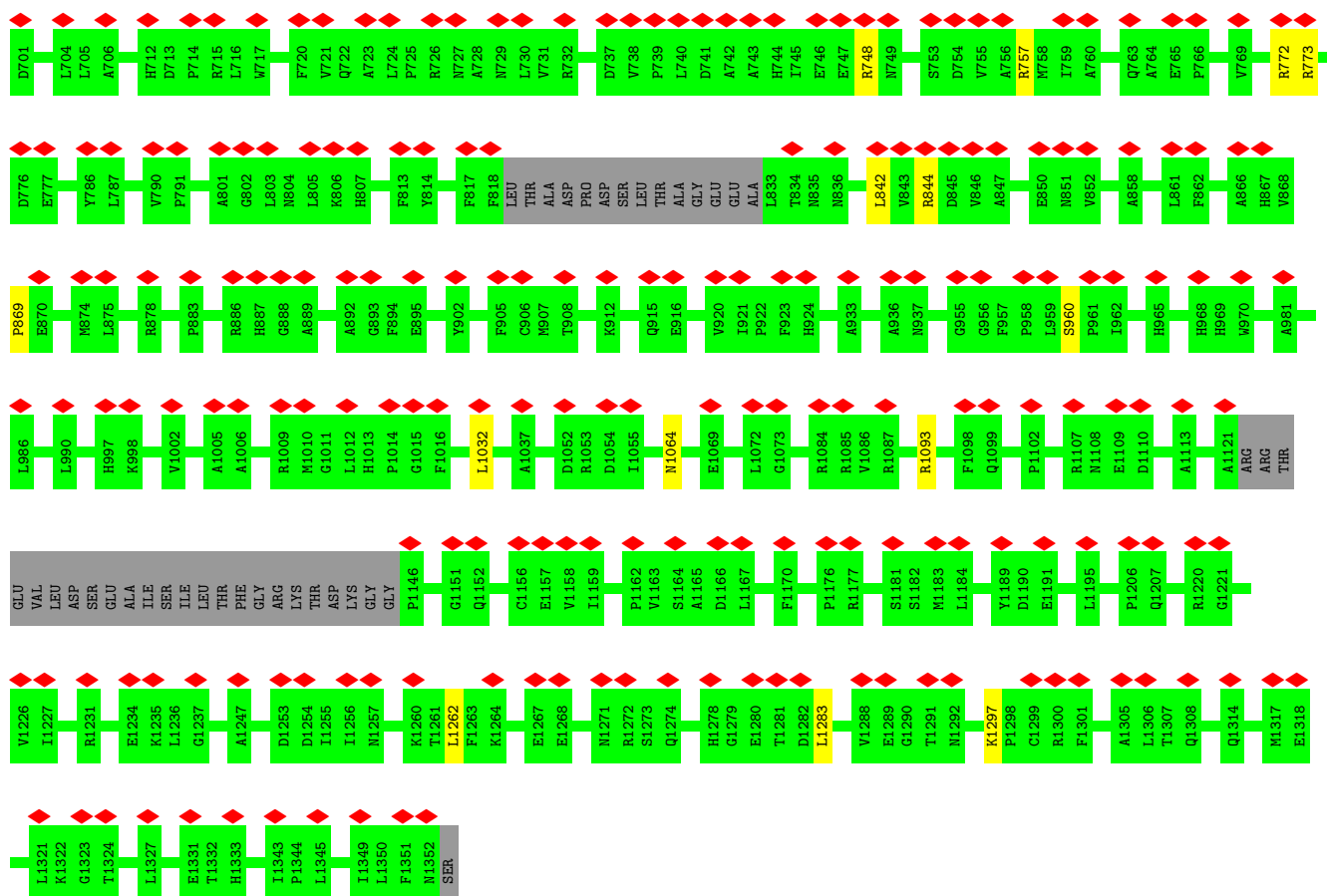
• Molecule 1: Major capsid protein



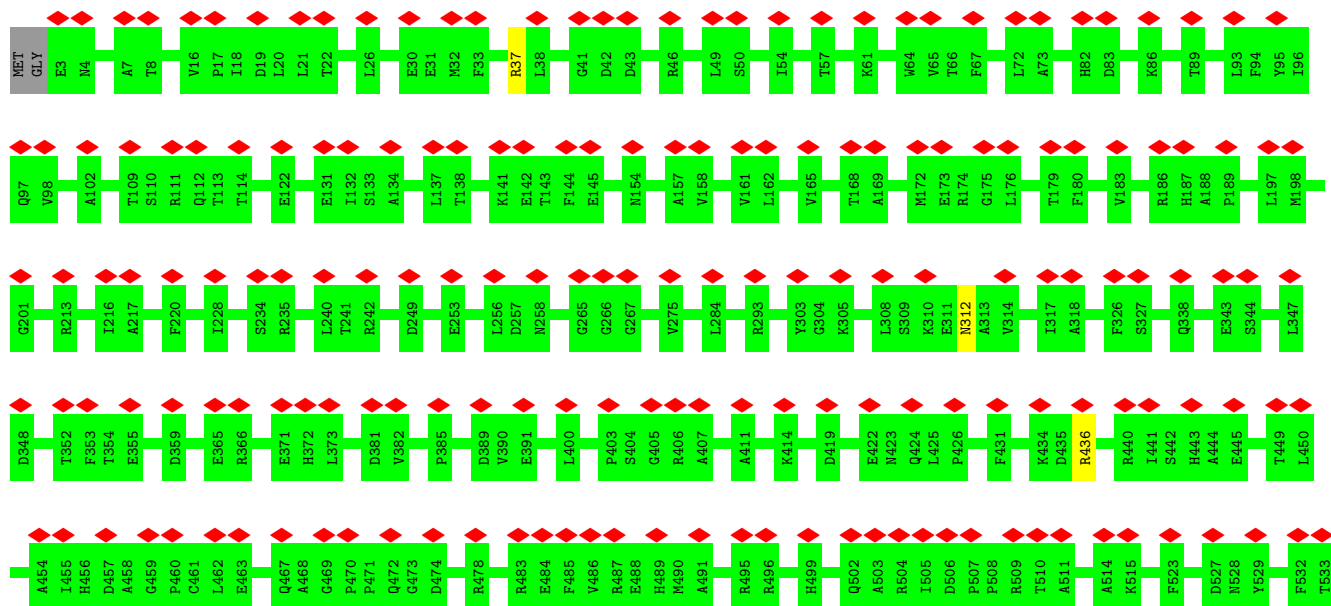


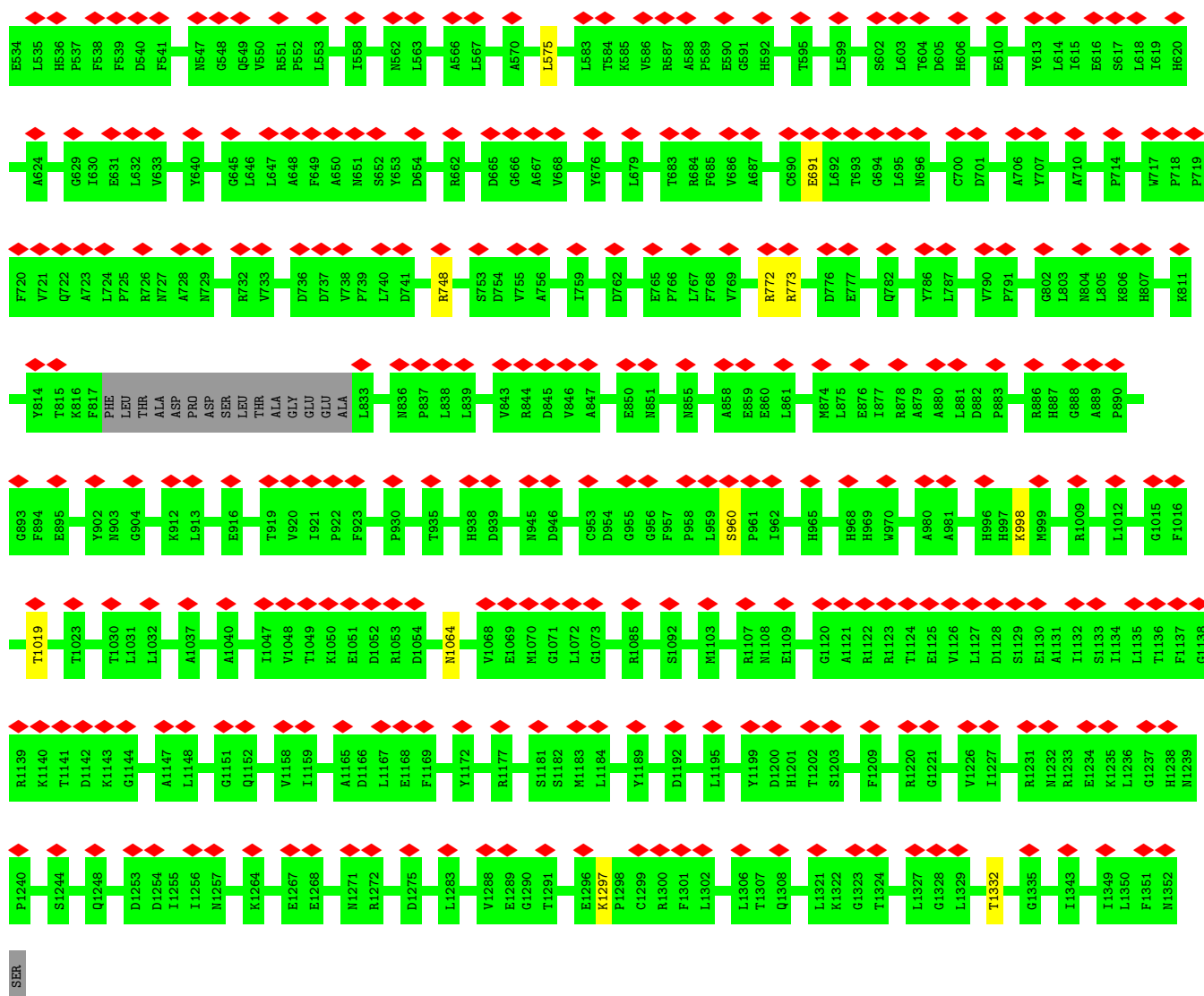
• Molecule 1: Major capsid protein



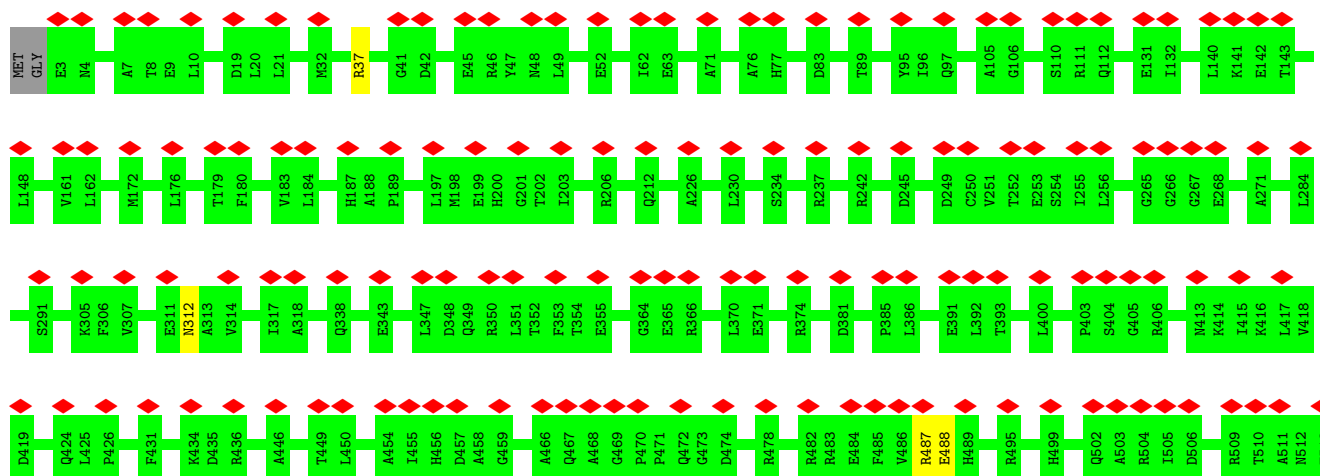


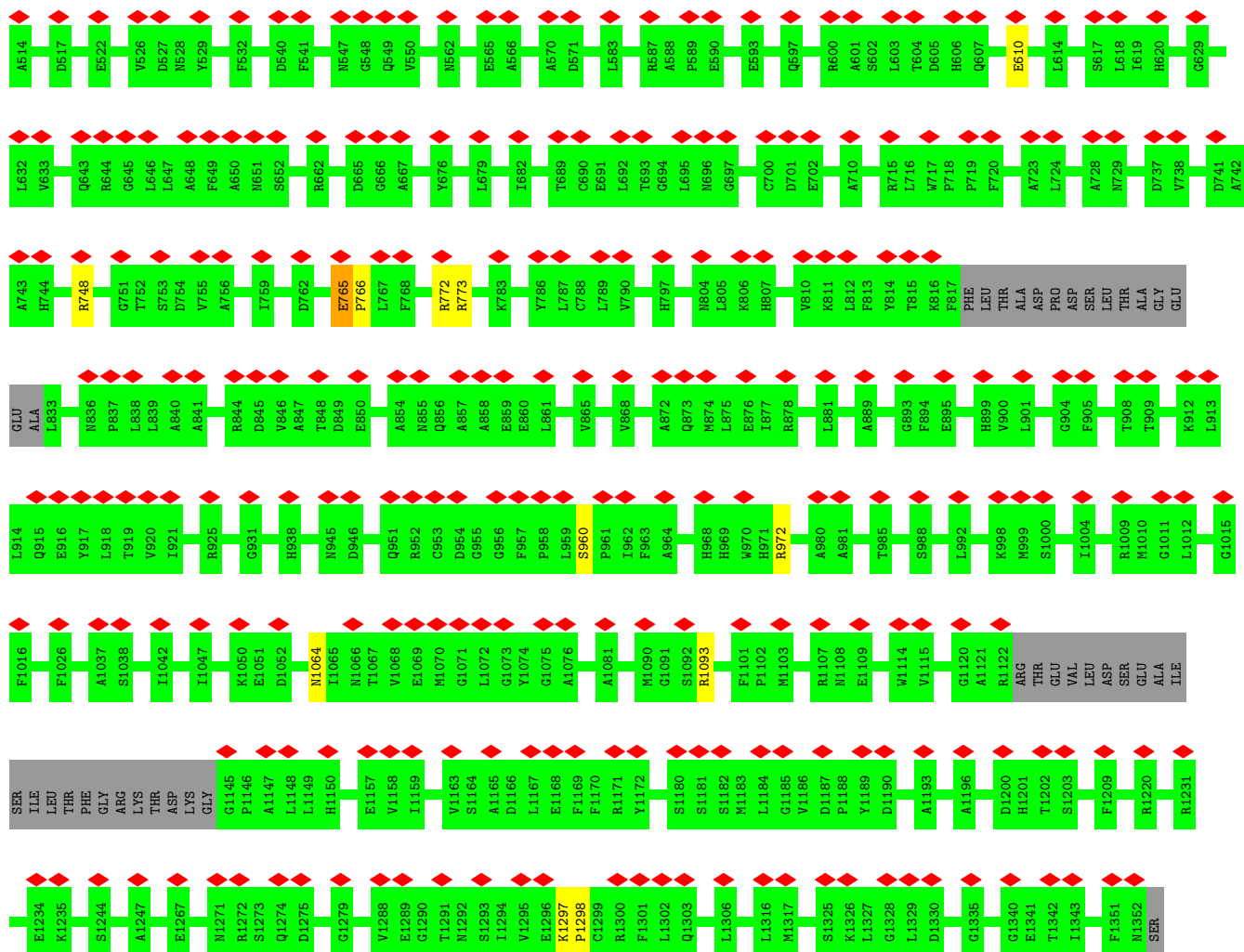
• Molecule 1: Major capsid protein



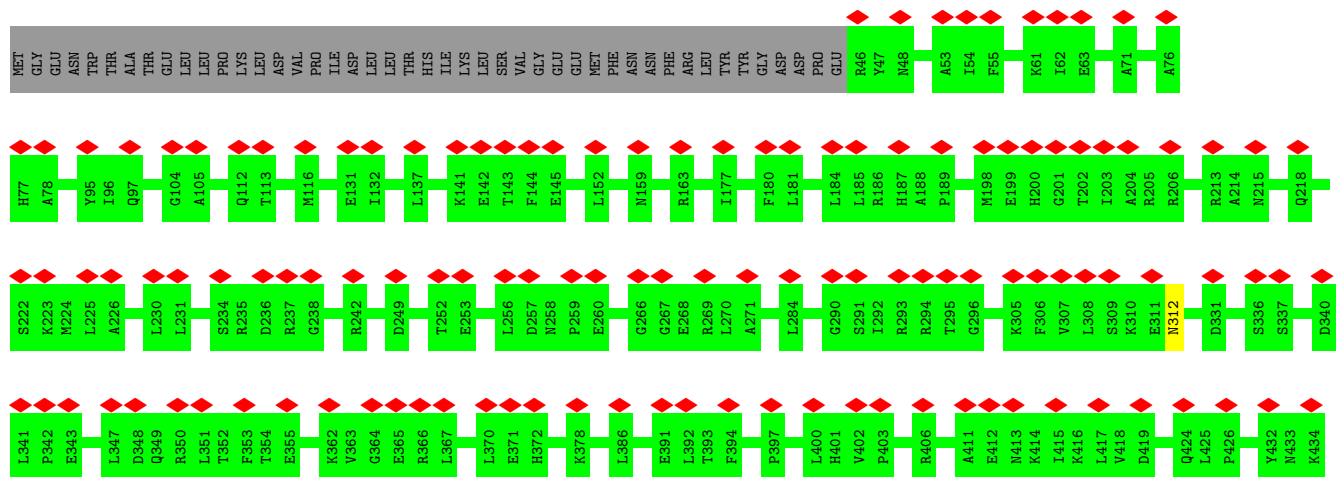


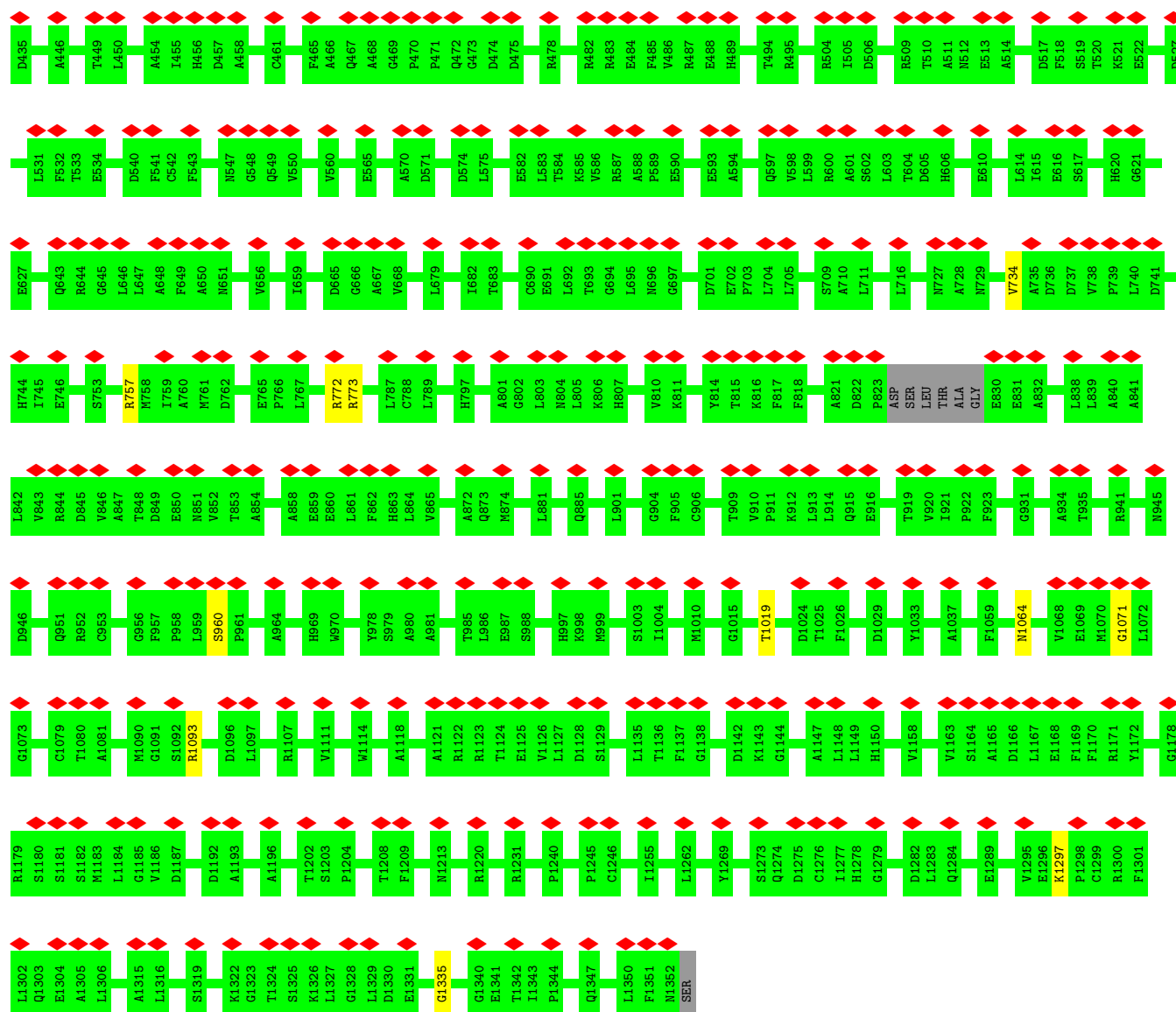
• Molecule 1: Major capsid protein



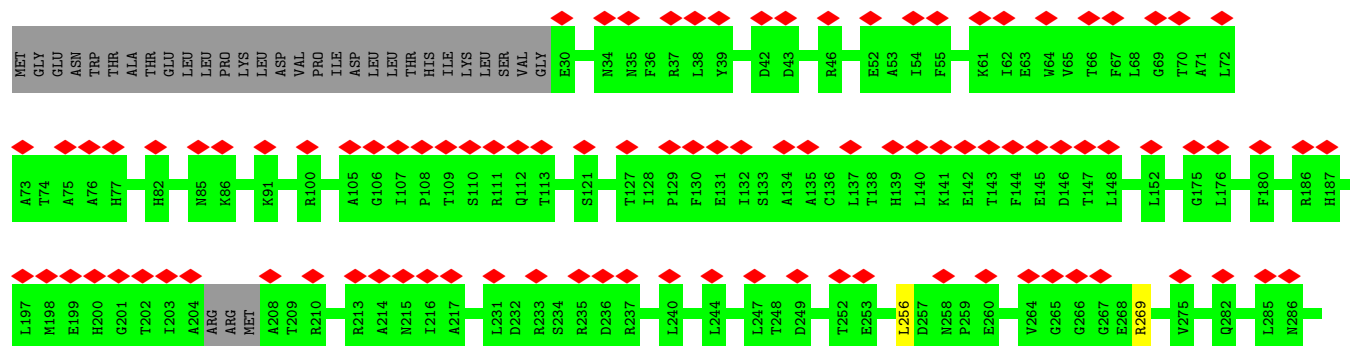
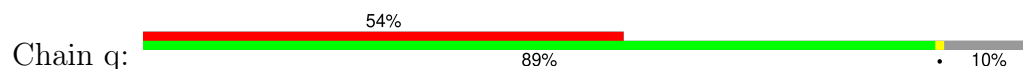


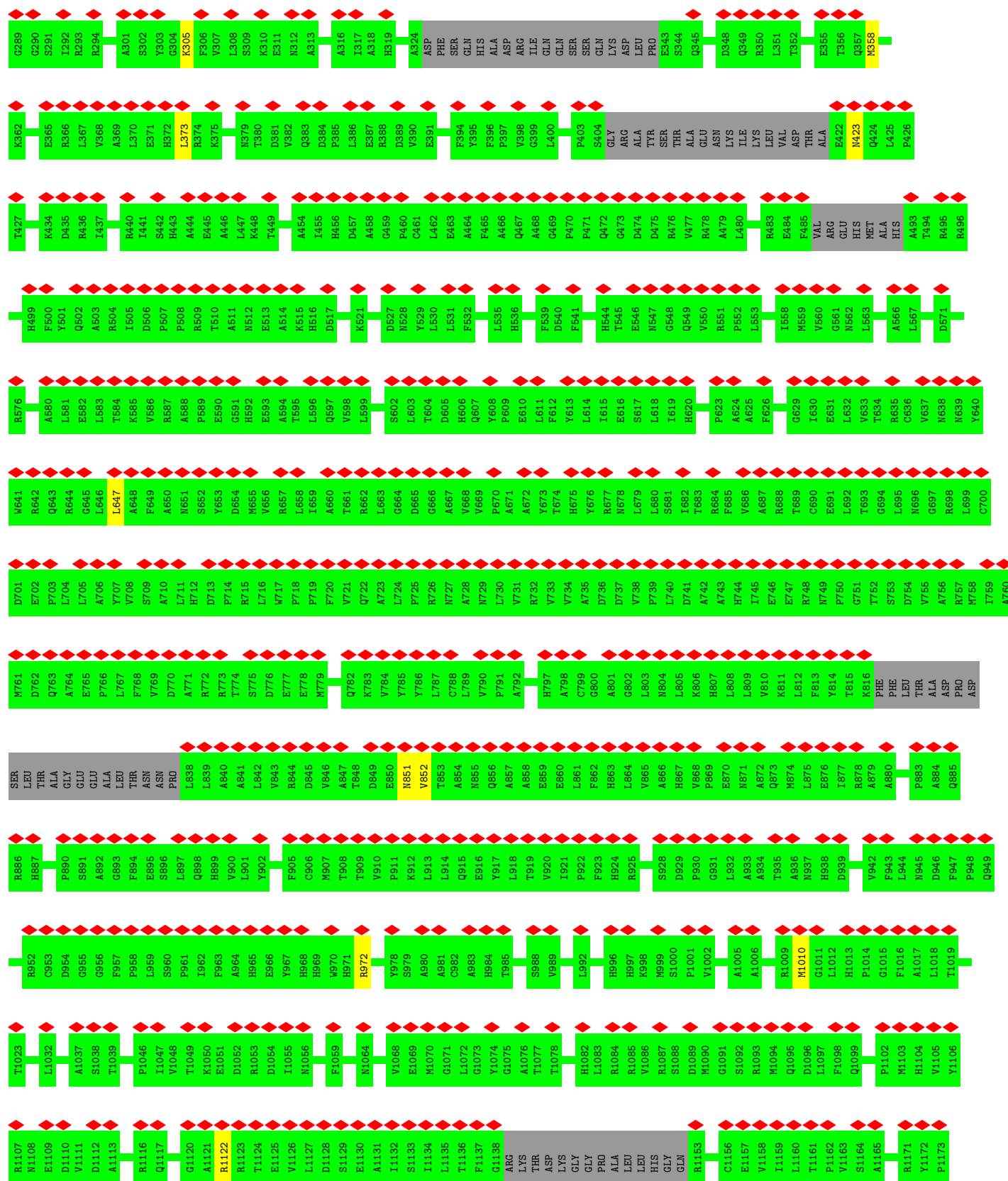
• Molecule 1: Major capsid protein

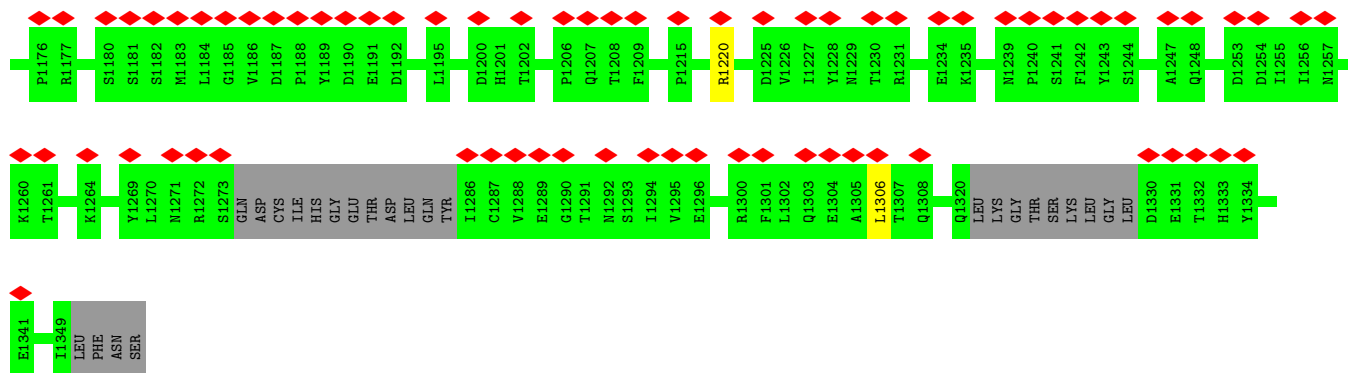




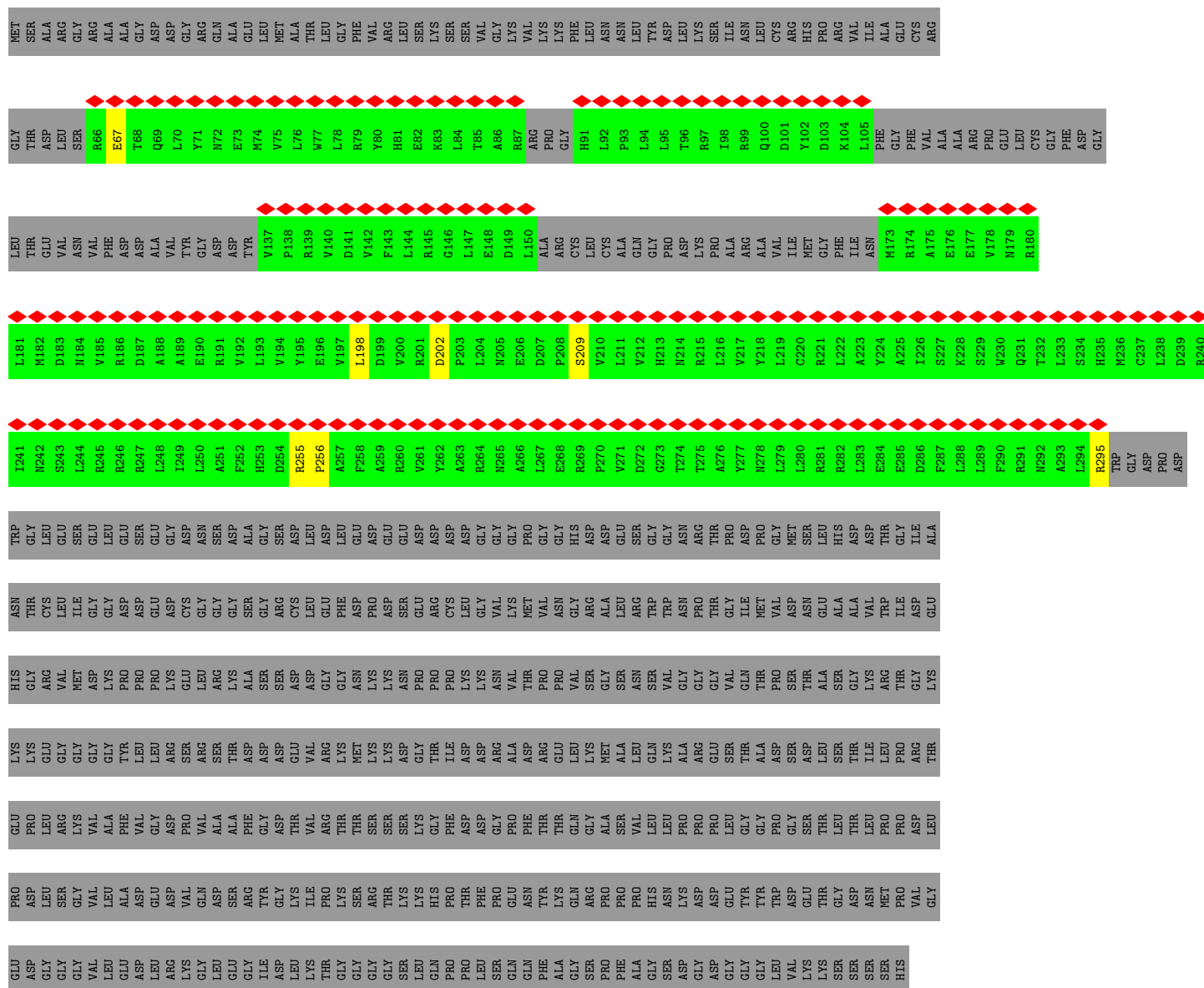
• Molecule 1: Major capsid protein



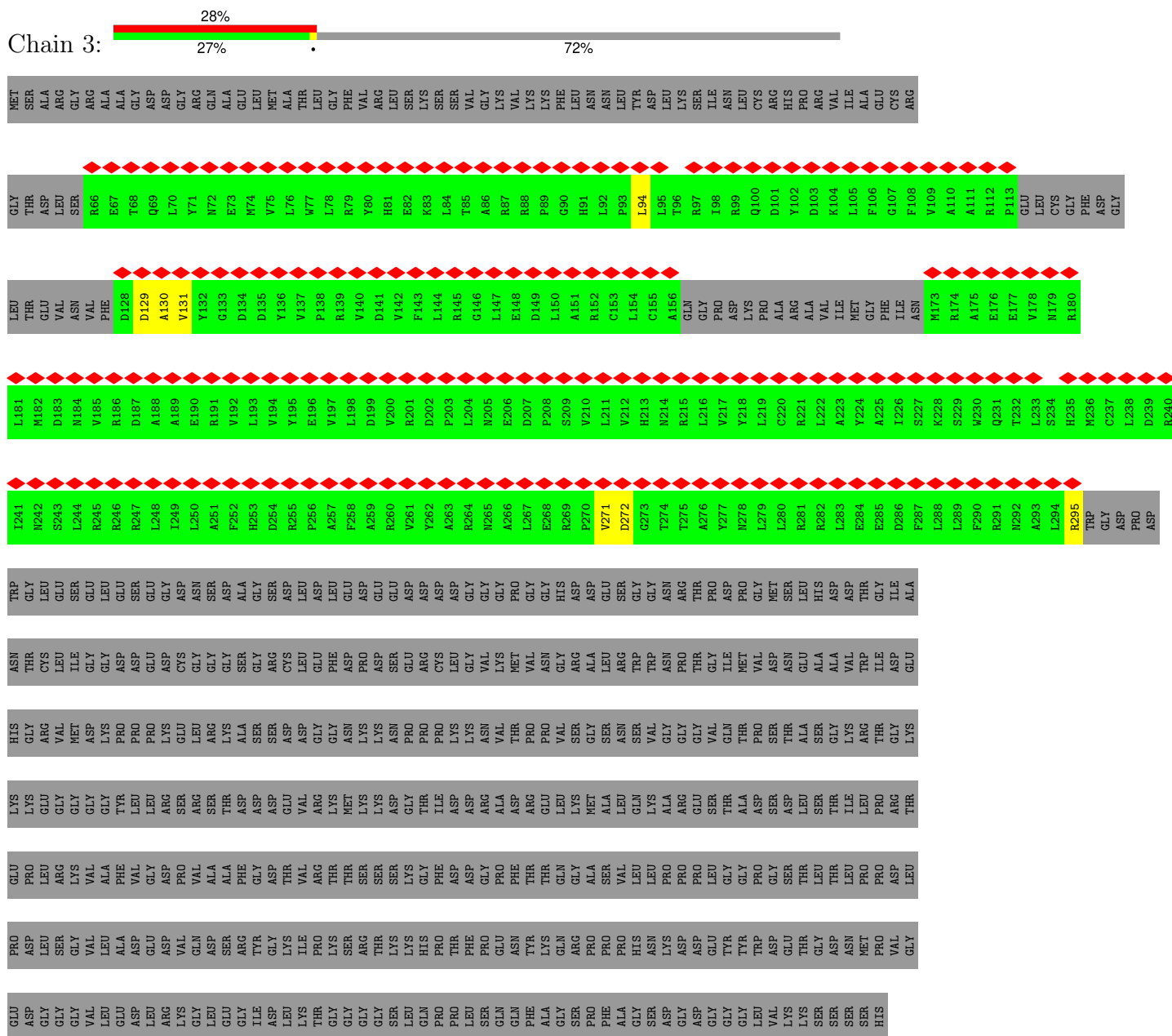




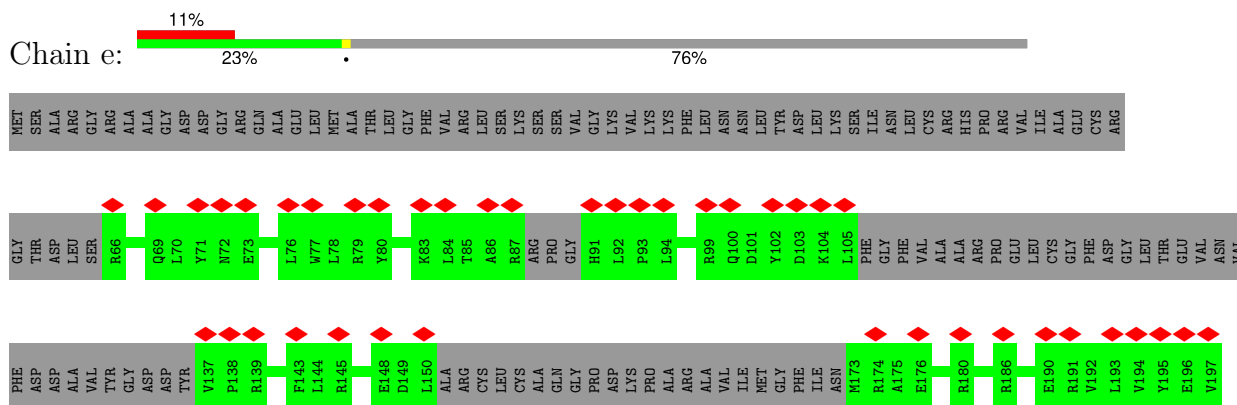
• Molecule 2: Tegument protein

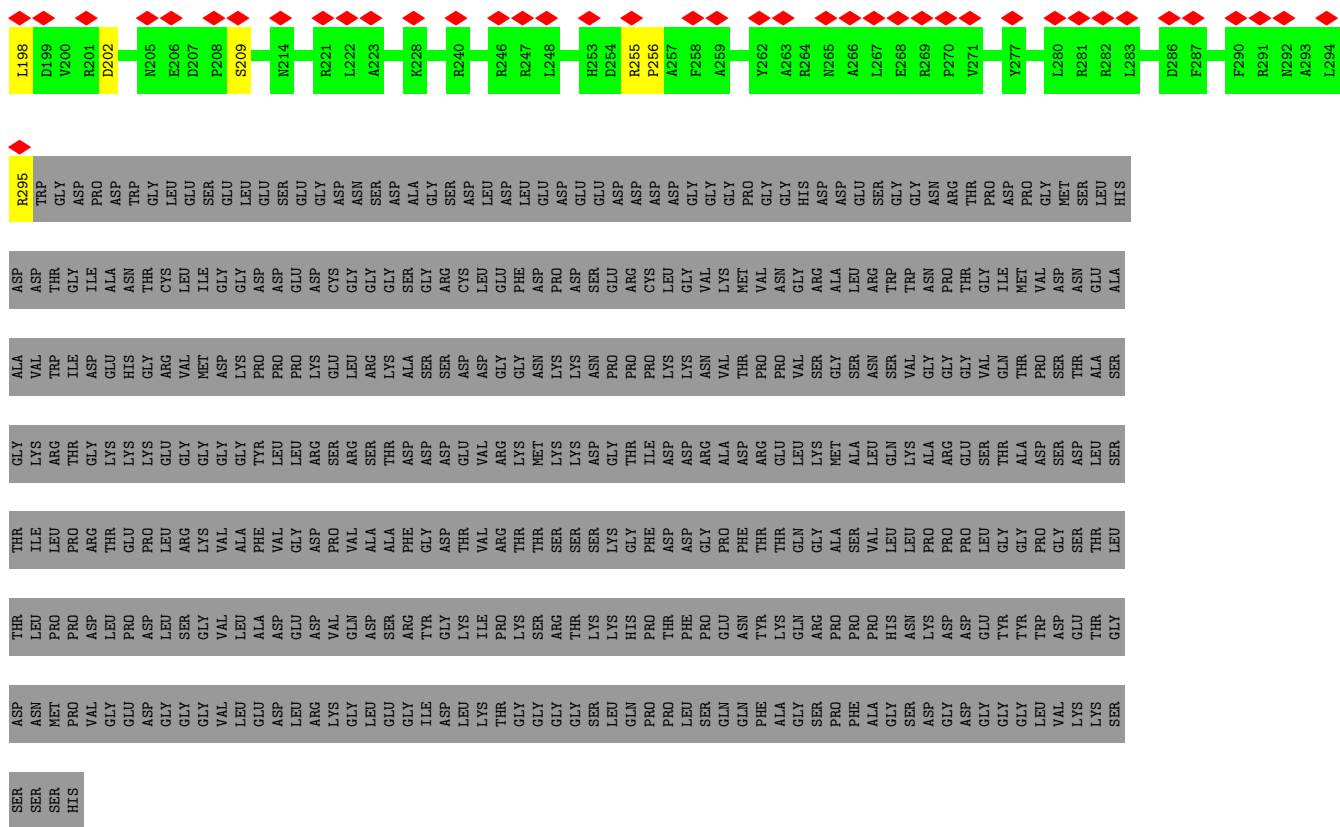


• Molecule 2: Tegument protein

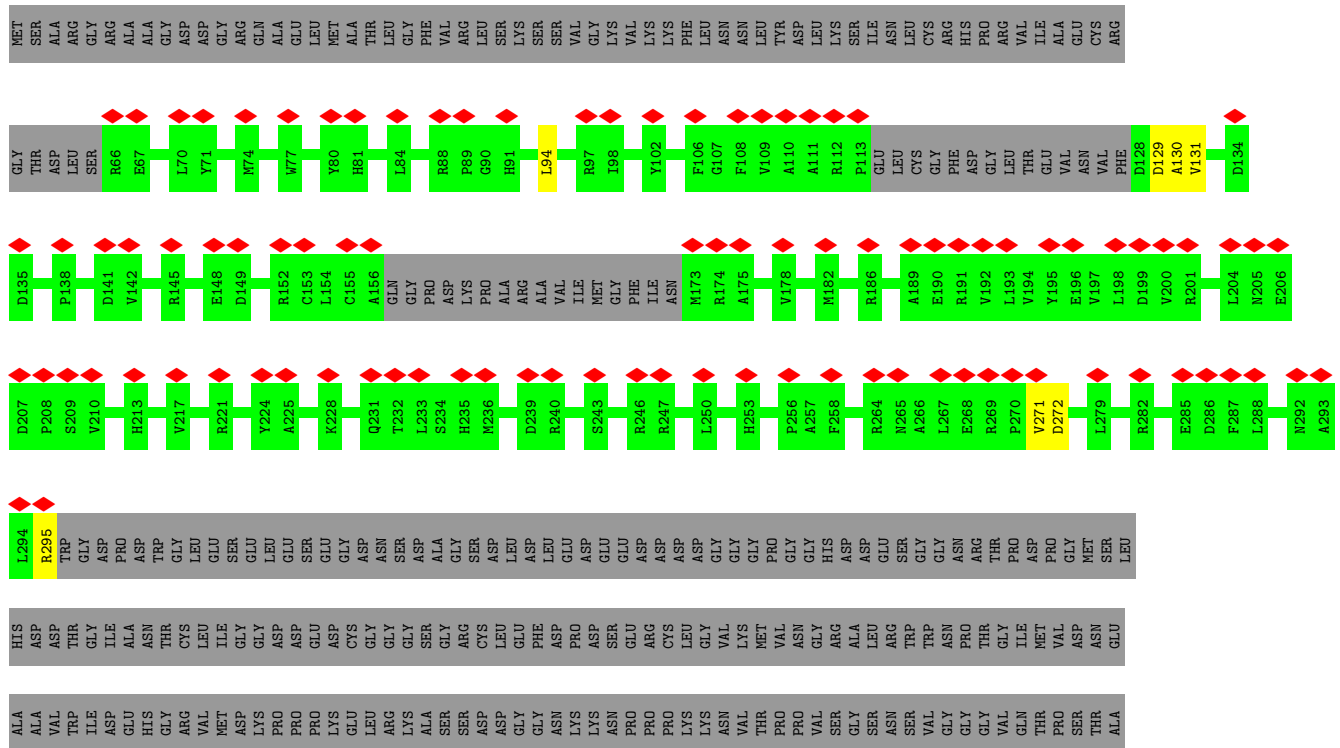


- Molecule 2: Tegument protein

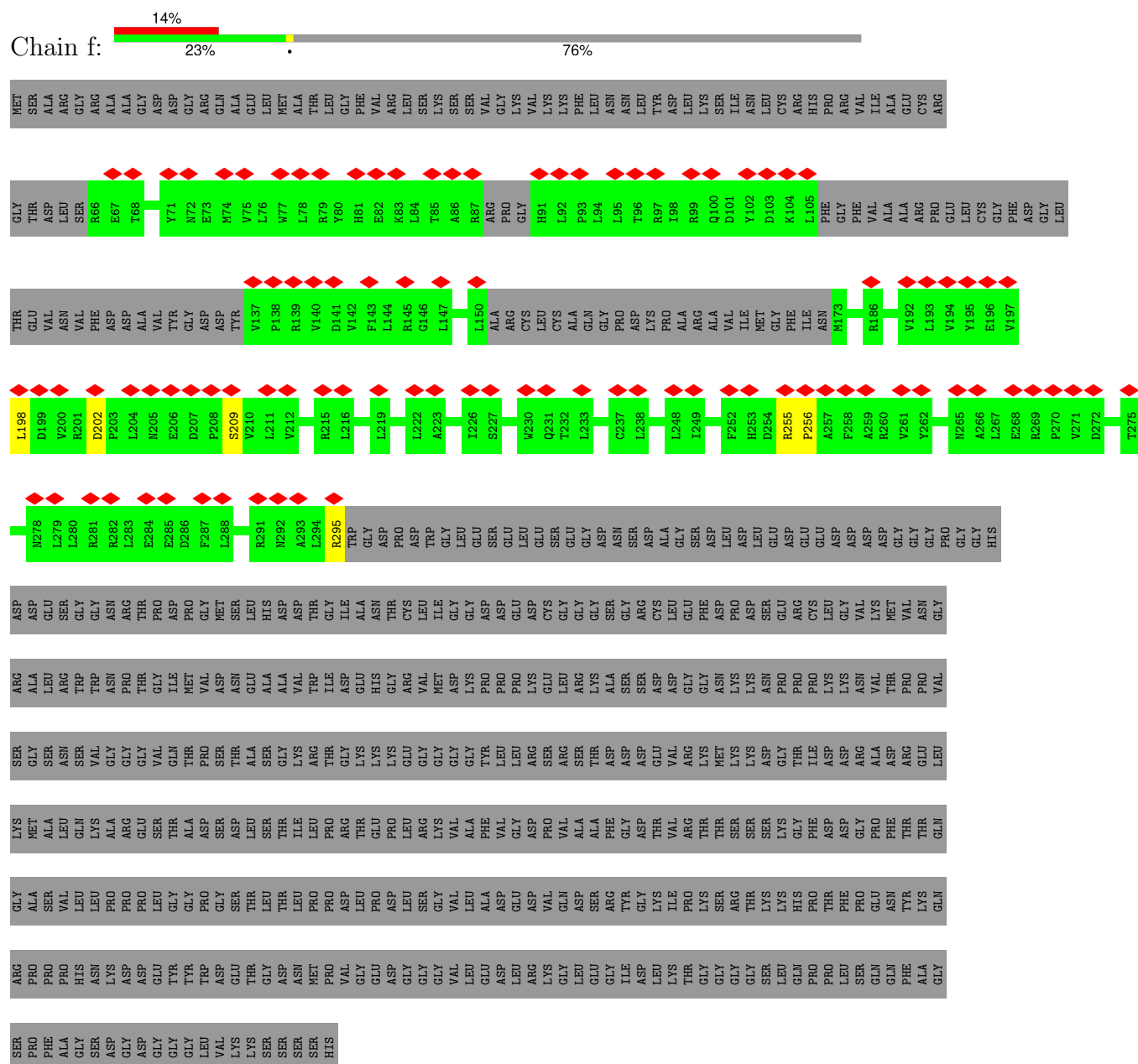




- Molecule 2: Tegument protein



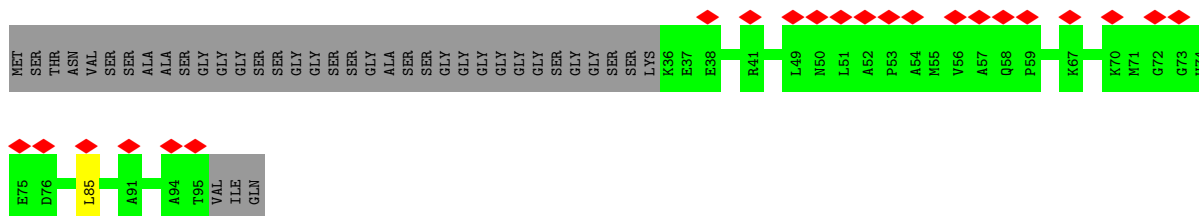
- Molecule 2: Tegument protein



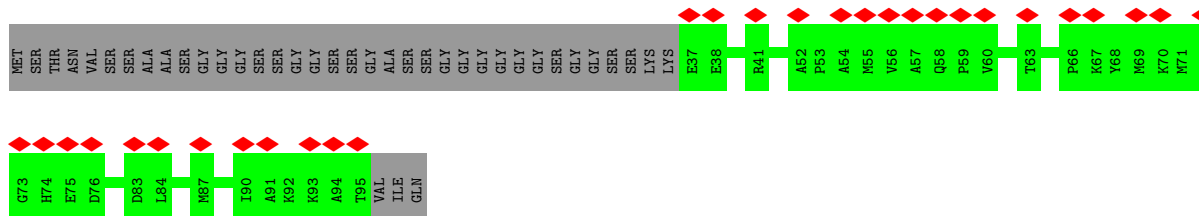


GLY	GLY	GLU	LEU	SER	VAL	GLY	PRO
GLY	GLY	TYR	GLY	THR	THR	THR	ASP
LEU	LEU	TRP	PRO	ASP	ALA	ALA	THR
VAL	VAL	ASP	GLY	SER	SER	ASP	SER
LYS	LYS	GLU	SER	ASP	LEU	ALA	SER
LYS	SER	THR	THR	LEU	SER	GLY	LEU
SER	SER	GLY	LEU	SER	THR	SER	ALA
SER	SER	ASP	THR	THR	THR	GLY	ALA
SER	SER	ASN	LEU	ILE	ILE	LYS	ASP
SER	SER	MET	LEU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

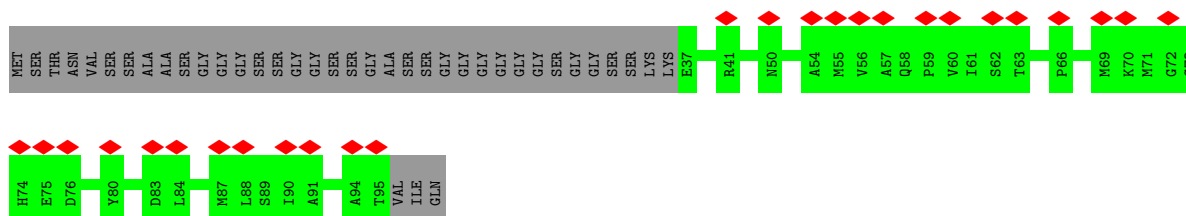
- Molecule 3: Small capsomere-interacting protein



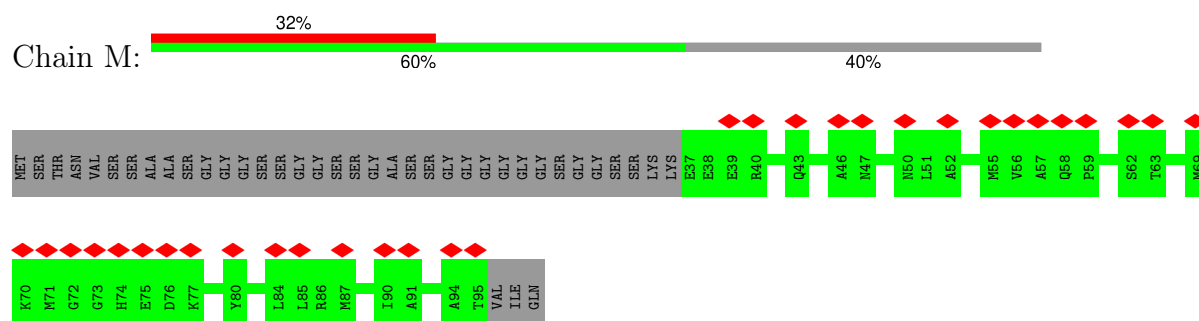
- Molecule 3: Small capsomere-interacting protein



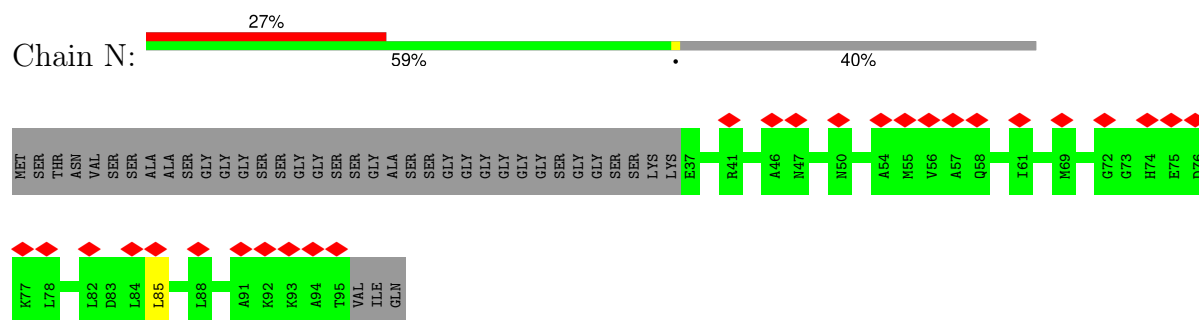
- Molecule 3: Small capsomere-interacting protein



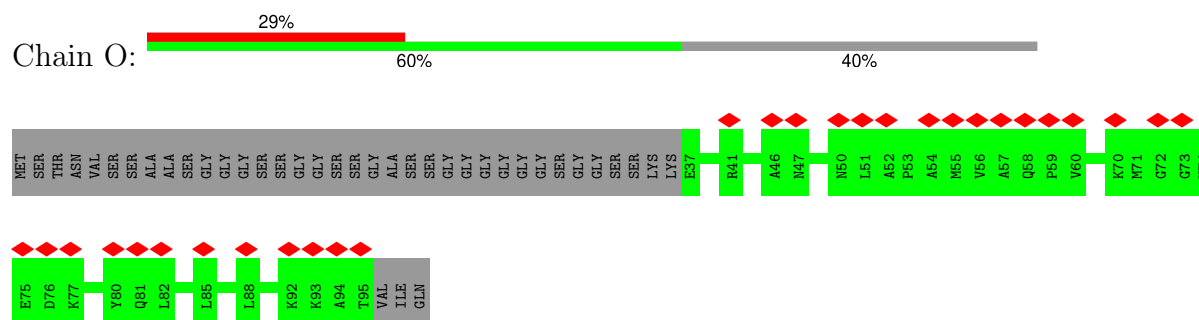
- Molecule 3: Small capsomere-interacting protein



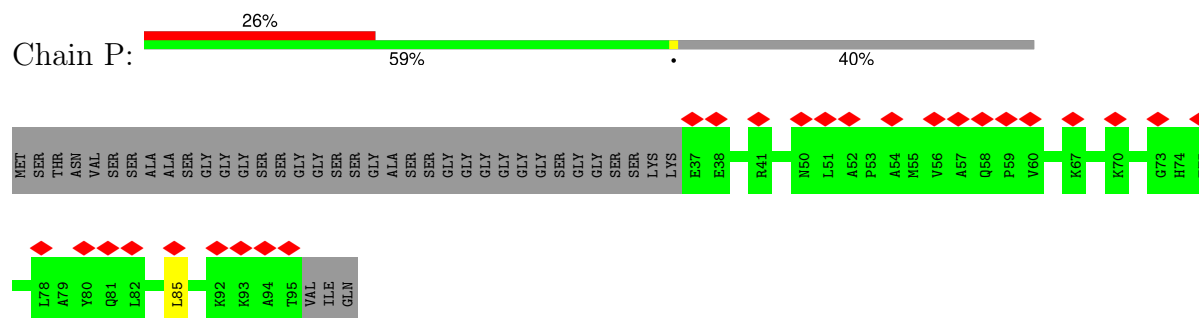
- Molecule 3: Small capsomere-interacting protein



- Molecule 3: Small capsomere-interacting protein

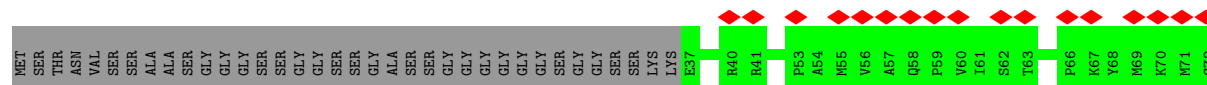


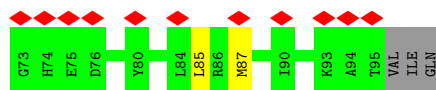
- Molecule 3: Small capsomere-interacting protein



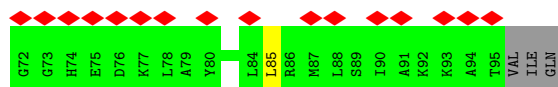
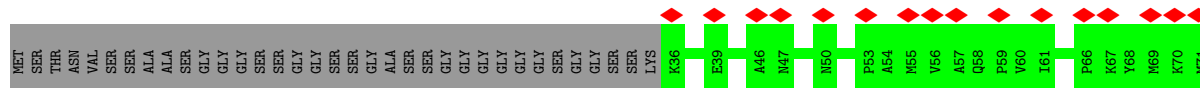
- Molecule 3: Small capsomere-interacting protein



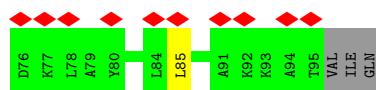




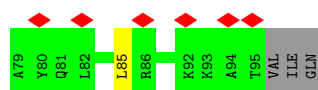
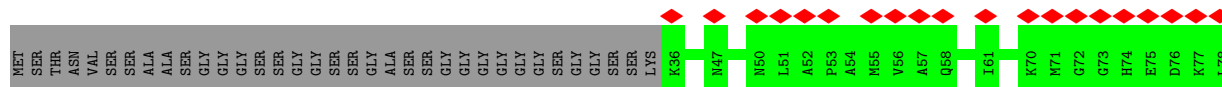
- Molecule 3: Small capsomere-interacting protein



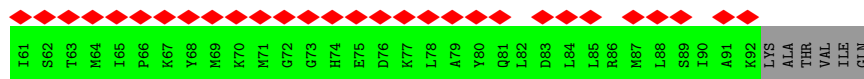
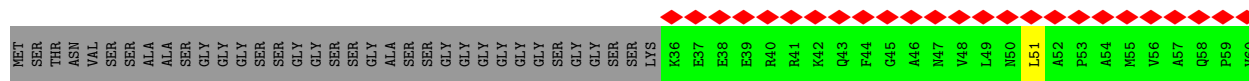
- Molecule 3: Small capsomere-interacting protein




- Molecule 3: Small capsomere-interacting protein

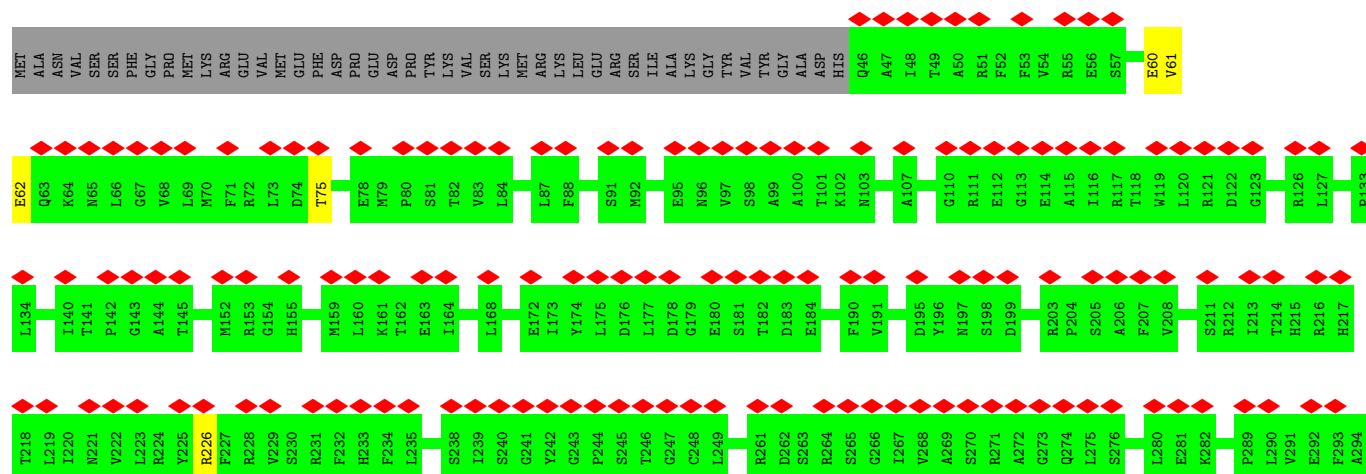


- Molecule 3: Small capsomere-interacting protein

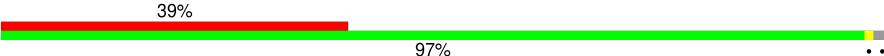


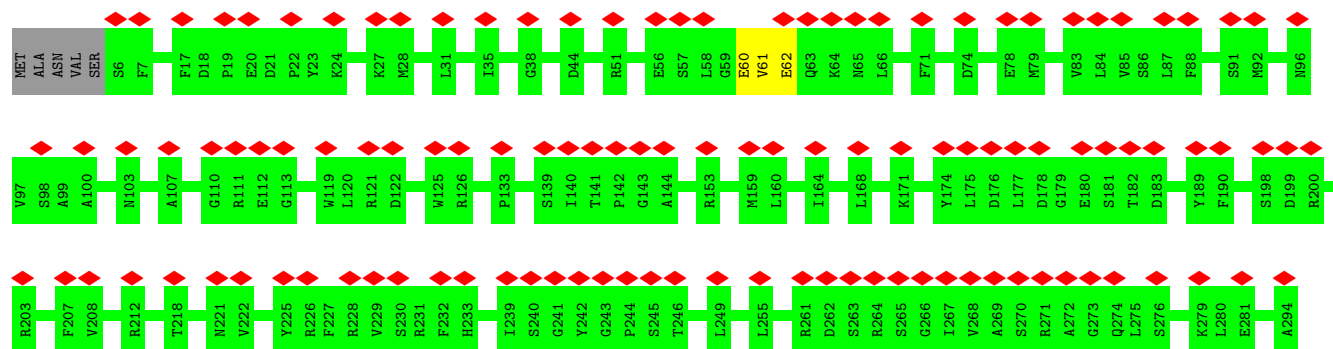
- Molecule 4: Minor capsid protein

Chain y: 

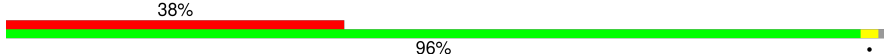


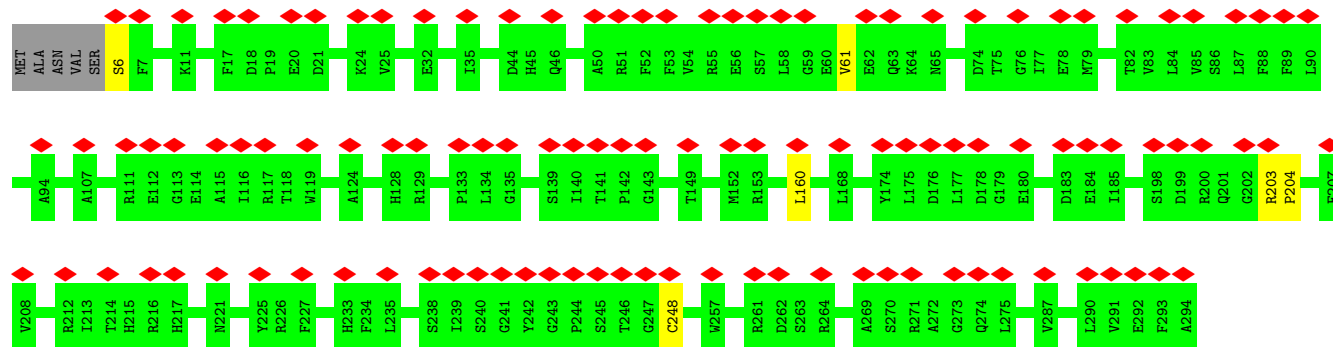
• Molecule 4: Minor capsid protein

Chain S: 



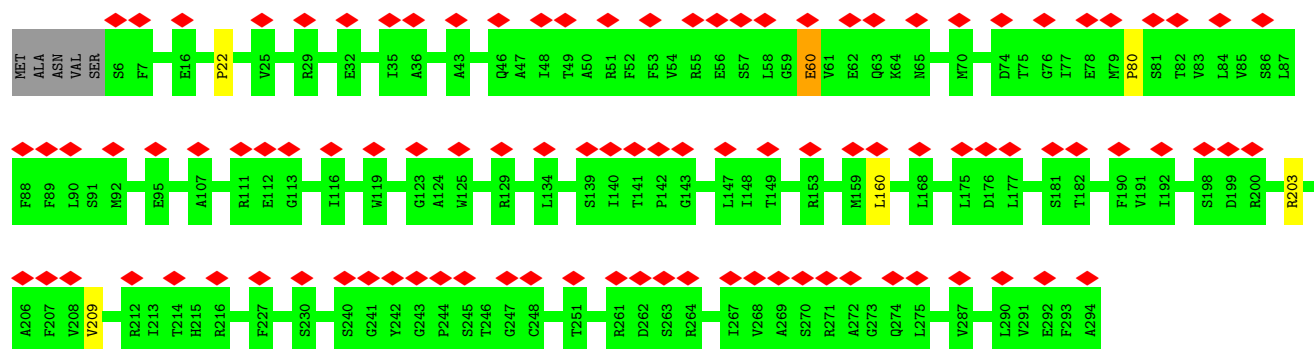
• Molecule 4: Minor capsid protein

Chain T: 



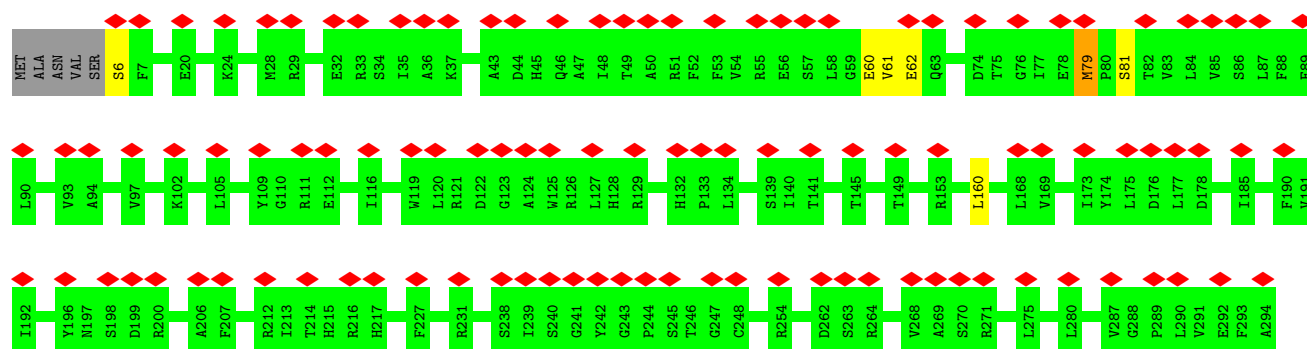
• Molecule 4: Minor capsid protein

Chain U: 



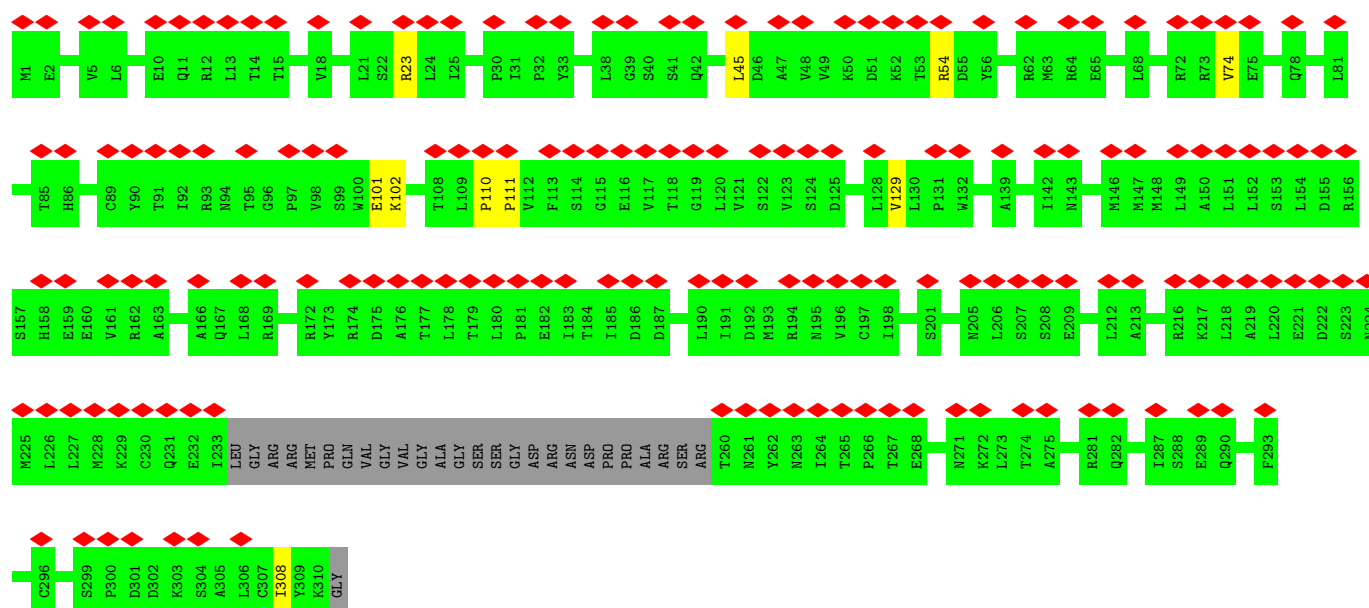
• Molecule 4: Minor capsid protein

Chain V: 37% 96%

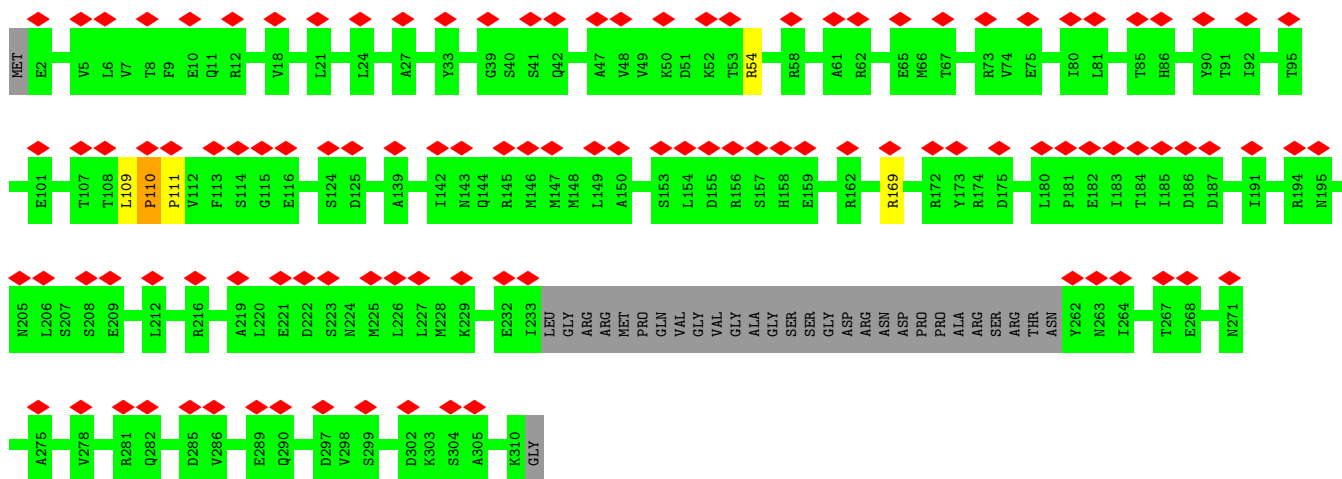
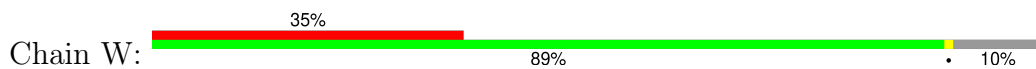


• Molecule 5: Triplex capsid protein 2

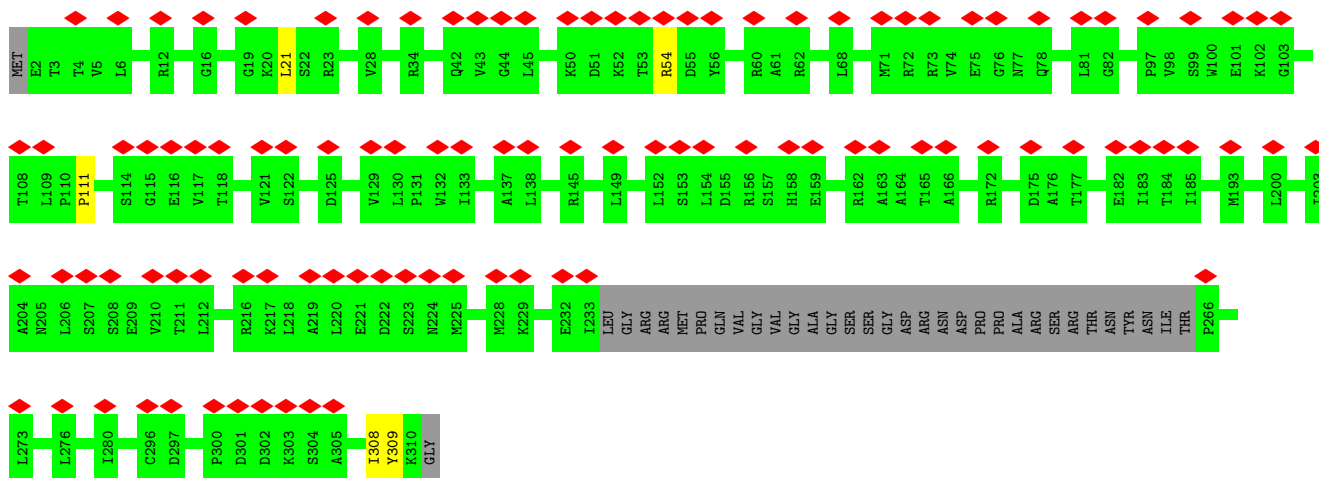
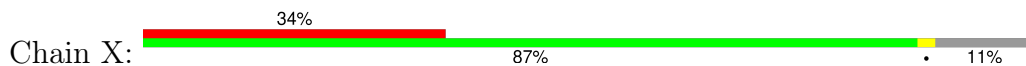
Chain z: 53% 88% 9%



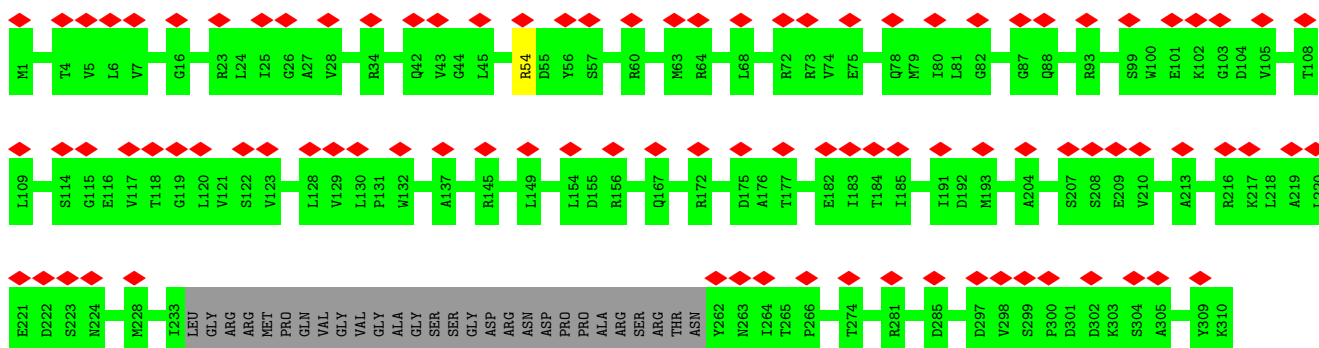
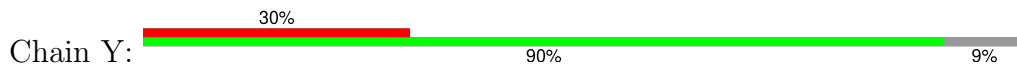
• Molecule 5: Triplex capsid protein 2



• Molecule 5: Triplex capsid protein 2




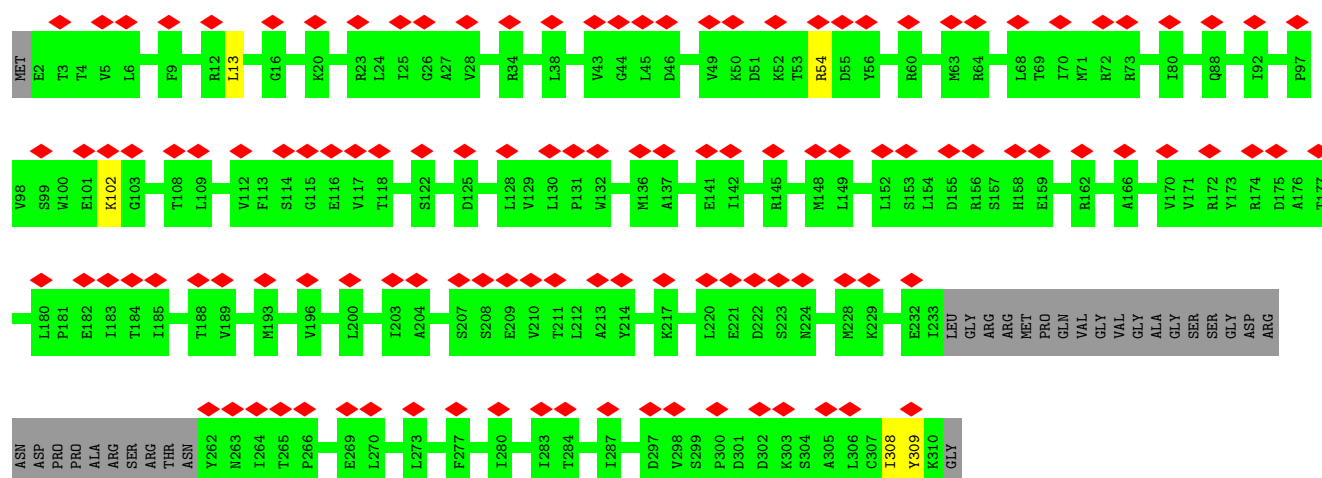
• Molecule 5: Triplex capsid protein 2




GLY

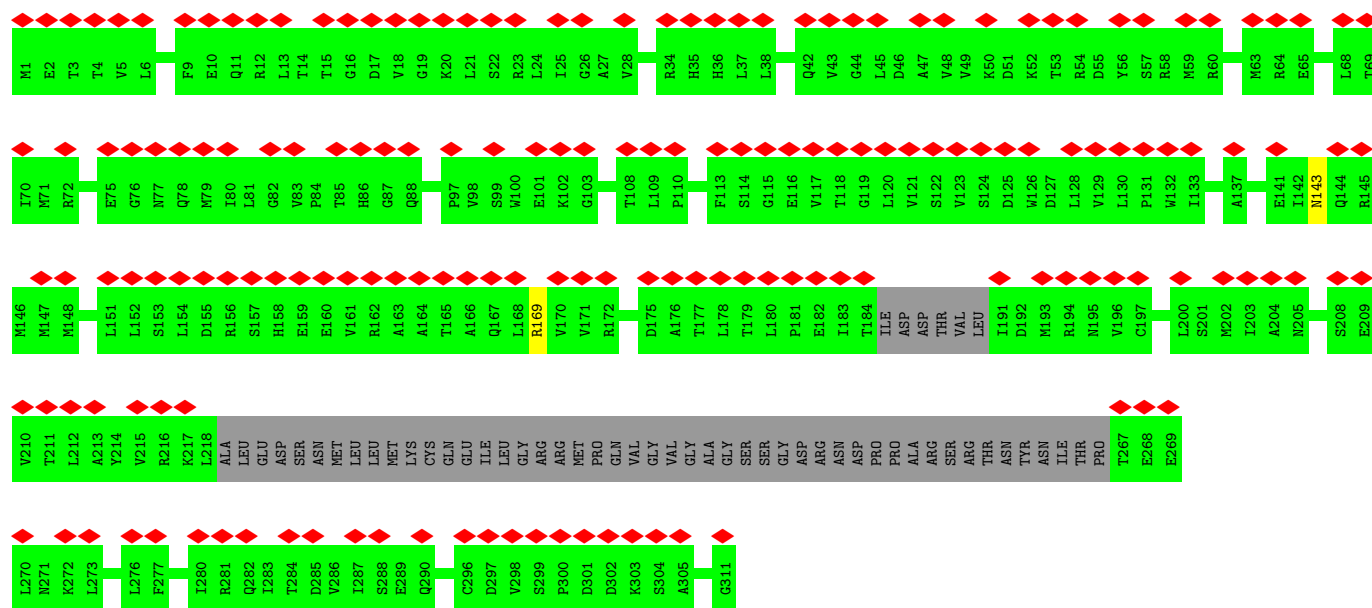
- Molecule 5: Triplex capsid protein 2

Chain Z: 




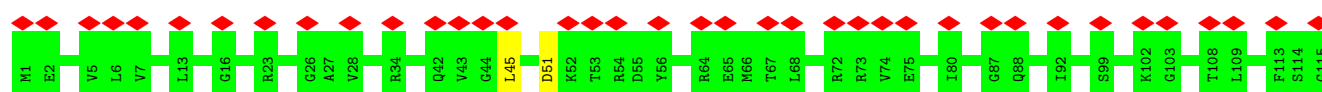
- Molecule 5: Triplex capsid protein 2

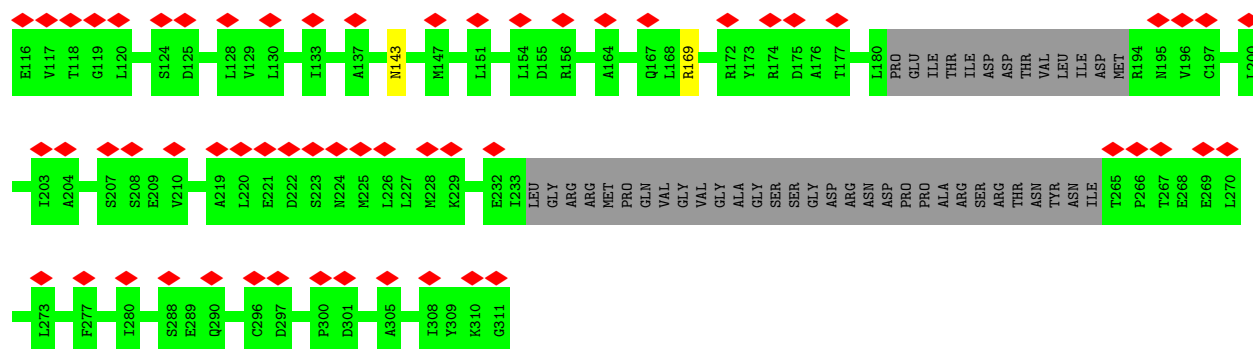
Chain 1: 



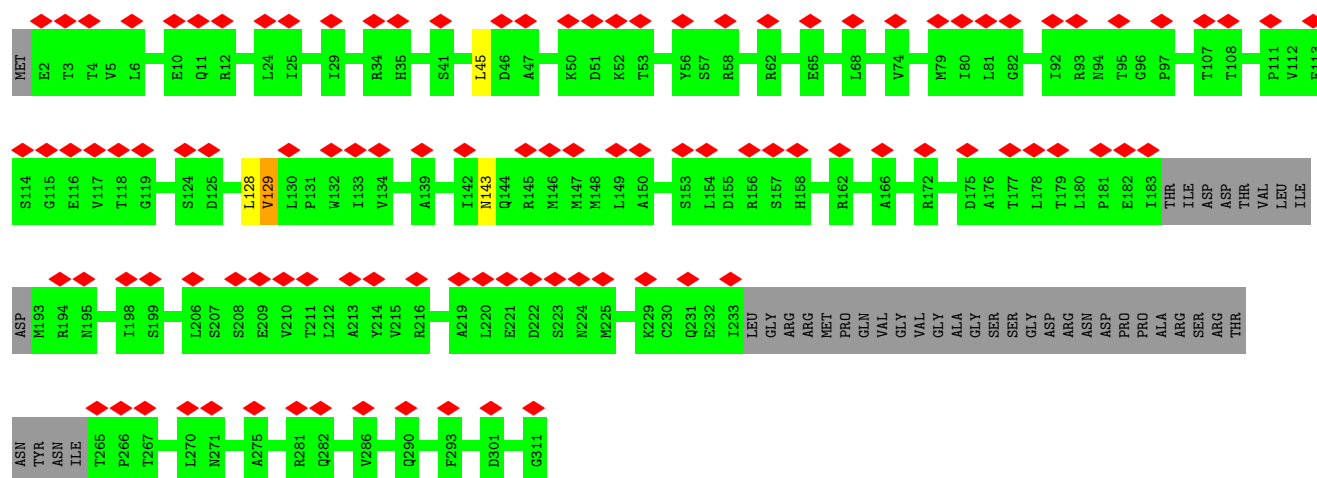
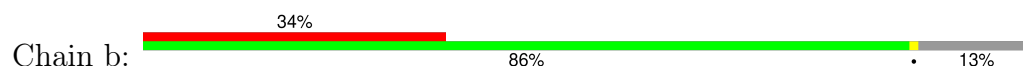
- Molecule 5: Triplex capsid protein 2

Chain a: 

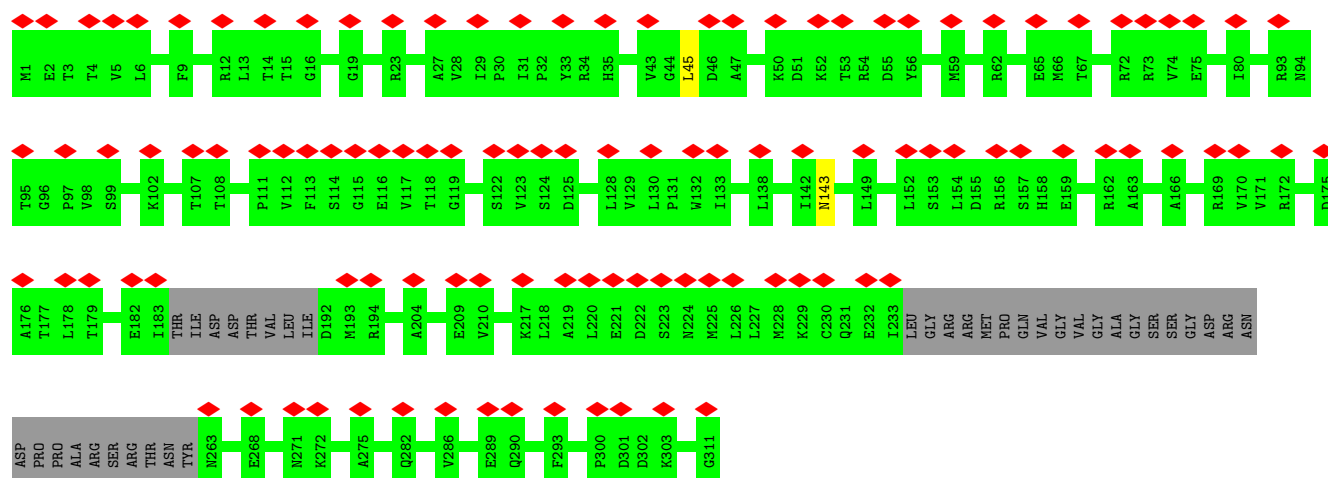
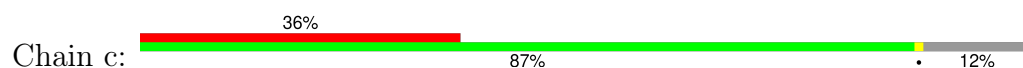




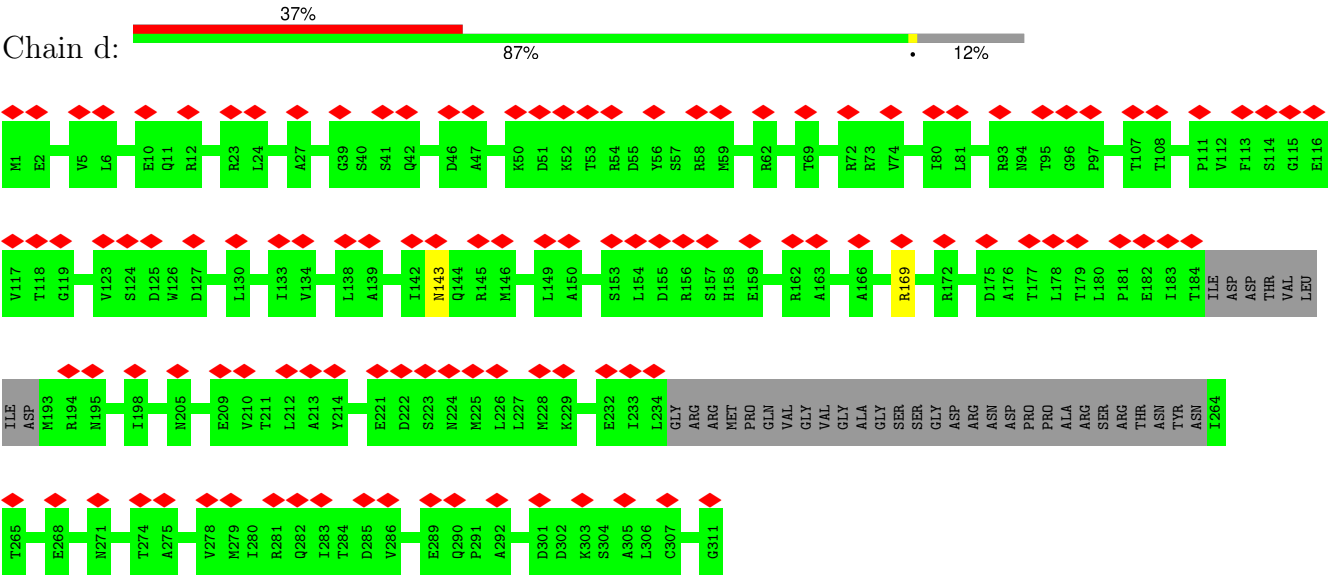
• Molecule 5: Triplex capsid protein 2



• Molecule 5: Triplex capsid protein 2



• Molecule 5: 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	47982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	47000	Depositor
Image detector	AGFA SCIENTA FILM	Depositor
Maximum map value	13.184	Depositor
Minimum map value	-7.318	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size (Å)	1729.2799, 1729.2799, 1729.2799	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.351, 1.351, 1.351	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	0.40	0/10779	0.63	0/14662
1	B	0.42	0/10591	0.63	0/14408
1	C	0.47	0/10590	0.66	0/14407
1	D	0.46	0/10615	0.66	0/14442
1	E	0.35	0/10735	0.61	0/14602
1	F	0.40	0/10648	0.63	0/14488
1	G	0.47	0/10823	0.67	0/14724
1	H	0.41	0/10823	0.64	0/14724
1	I	0.38	0/10662	0.62	0/14506
1	k	0.40	0/10445	0.64	0/14213
1	l	0.40	0/10790	0.65	2/14677 (0.0%)
1	m	0.41	0/10604	0.65	0/14426
1	n	0.36	0/10779	0.65	0/14662
1	o	0.39	0/10607	0.64	0/14430
1	p	0.38	0/10485	0.64	0/14261
1	q	0.35	0/9837	0.64	3/13377 (0.0%)
2	2	0.39	1/1493 (0.1%)	0.65	2/2016 (0.1%)
2	3	0.34	0/1696	0.59	0/2294
2	e	0.40	1/1493 (0.1%)	0.65	2/2016 (0.1%)
2	f	0.39	1/1493 (0.1%)	0.65	2/2016 (0.1%)
2	g	0.39	1/1493 (0.1%)	0.65	2/2016 (0.1%)
2	h	0.34	0/1696	0.59	0/2294
2	i	0.34	0/1696	0.59	0/2294
2	j	0.34	0/1696	0.59	0/2294
3	J	0.32	0/477	0.61	0/637
3	K	0.32	0/468	0.63	0/626
3	L	0.33	0/468	0.60	0/626
3	M	0.43	0/468	0.65	0/626
3	N	0.32	0/468	0.62	0/626
3	O	0.33	0/468	0.65	0/626
3	P	0.36	0/468	0.62	0/626
3	Q	0.33	0/468	0.60	0/626
3	R	0.33	0/468	0.65	0/626
3	r	0.33	0/477	0.68	0/637

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	s	0.32	0/468	0.63	0/626
3	t	0.33	0/468	0.63	0/626
3	u	0.32	0/477	0.62	0/637
3	v	0.32	0/477	0.62	0/637
3	w	0.34	0/477	0.68	0/637
3	x	0.34	0/456	0.70	1/609 (0.2%)
4	S	0.40	0/2357	0.63	0/3185
4	T	0.38	0/2357	0.66	4/3185 (0.1%)
4	U	0.37	0/2357	0.64	0/3185
4	V	0.36	0/2357	0.64	0/3185
4	y	0.42	0/2020	0.71	0/2735
5	1	0.34	0/2037	0.65	0/2761
5	W	0.32	0/2232	0.65	1/3031 (0.0%)
5	X	0.30	0/2196	0.60	0/2980
5	Y	0.34	0/2240	0.66	0/3041
5	Z	0.33	0/2232	0.64	0/3031
5	a	0.35	0/2113	0.62	0/2862
5	b	0.31	0/2138	0.60	0/2897
5	c	0.35	0/2170	0.62	0/2940
5	d	0.36	0/2169	0.61	0/2939
5	z	0.35	1/2255 (0.0%)	0.67	1/3062 (0.0%)
All	All	0.39	5/223320 (0.0%)	0.64	20/303322 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	T	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	209	SER	C-N	9.91	1.56	1.34
2	2	209	SER	C-N	9.90	1.56	1.34
2	g	209	SER	C-N	9.89	1.56	1.34
2	f	209	SER	C-N	9.88	1.56	1.34
5	z	129	VAL	C-N	-5.37	1.21	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	209	SER	O-C-N	-11.48	104.33	122.70
2	f	209	SER	O-C-N	-11.48	104.34	122.70
2	2	209	SER	O-C-N	-11.47	104.35	122.70
2	g	209	SER	O-C-N	-11.46	104.36	122.70
5	W	110	PRO	C-N-CD	-8.26	102.42	120.60
2	e	209	SER	CA-C-N	8.05	134.91	117.20
2	f	209	SER	CA-C-N	8.04	134.89	117.20
2	g	209	SER	CA-C-N	8.03	134.86	117.20
2	2	209	SER	CA-C-N	8.02	134.85	117.20
1	l	749	ASN	C-N-CD	-7.91	103.21	120.60
1	q	256	LEU	CA-CB-CG	7.45	132.44	115.30
4	T	6	SER	C-N-CA	-7.38	103.24	121.70
4	T	6	SER	CA-C-N	-7.03	101.73	117.20
1	l	956	GLY	N-CA-C	-7.01	95.58	113.10
5	z	110	PRO	C-N-CD	-6.97	105.25	120.60
3	x	51	LEU	CA-CB-CG	6.51	130.27	115.30
1	q	647	LEU	CB-CG-CD1	-6.11	100.62	111.00
4	T	160	LEU	CA-CB-CG	6.01	129.12	115.30
4	T	6	SER	O-C-N	5.39	131.32	122.70
1	q	1306	LEU	CA-CB-CG	-5.10	103.58	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	T	203	ARG	Peptide
4	T	248	CYS	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	A	1331/1353 (98%)	1204 (90%)	126 (10%)	1 (0%)	48	83
1	B	1304/1353 (96%)	1209 (93%)	92 (7%)	3 (0%)	44	78
1	C	1304/1353 (96%)	1182 (91%)	119 (9%)	3 (0%)	44	78
1	D	1308/1353 (97%)	1184 (90%)	123 (9%)	1 (0%)	48	83
1	E	1326/1353 (98%)	1186 (89%)	138 (10%)	2 (0%)	44	78
1	F	1313/1353 (97%)	1216 (93%)	92 (7%)	5 (0%)	30	68
1	G	1337/1353 (99%)	1223 (92%)	112 (8%)	2 (0%)	48	83
1	H	1337/1353 (99%)	1193 (89%)	142 (11%)	2 (0%)	48	83
1	I	1315/1353 (97%)	1190 (90%)	123 (9%)	2 (0%)	44	78
1	k	1287/1353 (95%)	1164 (90%)	117 (9%)	6 (0%)	25	64
1	l	1332/1353 (98%)	1211 (91%)	120 (9%)	1 (0%)	48	83
1	m	1306/1353 (96%)	1175 (90%)	125 (10%)	6 (0%)	25	64
1	n	1331/1353 (98%)	1202 (90%)	128 (10%)	1 (0%)	48	83
1	o	1307/1353 (97%)	1173 (90%)	130 (10%)	4 (0%)	37	72
1	p	1297/1353 (96%)	1167 (90%)	127 (10%)	3 (0%)	44	78
1	q	1201/1353 (89%)	1058 (88%)	143 (12%)	0	100	100
2	2	166/718 (23%)	153 (92%)	9 (5%)	4 (2%)	5	27
2	3	194/718 (27%)	177 (91%)	13 (7%)	4 (2%)	5	30
2	e	166/718 (23%)	153 (92%)	10 (6%)	3 (2%)	7	34
2	f	166/718 (23%)	154 (93%)	9 (5%)	3 (2%)	7	34
2	g	166/718 (23%)	154 (93%)	9 (5%)	3 (2%)	7	34
2	h	194/718 (27%)	177 (91%)	13 (7%)	4 (2%)	5	30
2	i	194/718 (27%)	176 (91%)	14 (7%)	4 (2%)	5	30
2	j	194/718 (27%)	176 (91%)	14 (7%)	4 (2%)	5	30
3	J	58/98 (59%)	54 (93%)	4 (7%)	0	100	100
3	K	57/98 (58%)	55 (96%)	2 (4%)	0	100	100
3	L	57/98 (58%)	57 (100%)	0	0	100	100
3	M	57/98 (58%)	57 (100%)	0	0	100	100
3	N	57/98 (58%)	54 (95%)	3 (5%)	0	100	100
3	O	57/98 (58%)	56 (98%)	1 (2%)	0	100	100
3	P	57/98 (58%)	56 (98%)	1 (2%)	0	100	100
3	Q	57/98 (58%)	54 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	57/98 (58%)	56 (98%)	1 (2%)	0	100	100
3	r	58/98 (59%)	57 (98%)	1 (2%)	0	100	100
3	s	57/98 (58%)	55 (96%)	2 (4%)	0	100	100
3	t	57/98 (58%)	56 (98%)	1 (2%)	0	100	100
3	u	58/98 (59%)	54 (93%)	4 (7%)	0	100	100
3	v	58/98 (59%)	56 (97%)	2 (3%)	0	100	100
3	w	58/98 (59%)	56 (97%)	2 (3%)	0	100	100
3	x	55/98 (56%)	52 (94%)	3 (6%)	0	100	100
4	S	287/294 (98%)	254 (88%)	30 (10%)	3 (1%)	13	49
4	T	287/294 (98%)	255 (89%)	30 (10%)	2 (1%)	19	56
4	U	287/294 (98%)	256 (89%)	28 (10%)	3 (1%)	13	49
4	V	287/294 (98%)	242 (84%)	40 (14%)	5 (2%)	7	35
4	y	247/294 (84%)	211 (85%)	33 (13%)	3 (1%)	11	44
5	l	251/311 (81%)	233 (93%)	17 (7%)	1 (0%)	30	68
5	W	277/311 (89%)	239 (86%)	36 (13%)	2 (1%)	19	56
5	X	273/311 (88%)	250 (92%)	21 (8%)	2 (1%)	19	56
5	Y	278/311 (89%)	251 (90%)	27 (10%)	0	100	100
5	Z	277/311 (89%)	253 (91%)	23 (8%)	1 (0%)	30	68
5	a	261/311 (84%)	241 (92%)	20 (8%)	0	100	100
5	b	264/311 (85%)	249 (94%)	14 (5%)	1 (0%)	30	68
5	c	268/311 (86%)	248 (92%)	20 (8%)	0	100	100
5	d	268/311 (86%)	253 (94%)	15 (6%)	0	100	100
5	z	280/311 (90%)	255 (91%)	23 (8%)	2 (1%)	19	56
All	All	27383/33540 (82%)	24832 (91%)	2455 (9%)	96 (0%)	32	68

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	692	LEU
1	E	960	SER
1	k	1262	LEU
1	l	750	PRO
1	m	148	LEU
1	m	1262	LEU

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Mol	Chain	Res	Type
1	o	610	GLU
2	2	198	LEU
2	2	256	PRO
2	3	130	ALA
2	e	198	LEU
2	e	256	PRO
2	h	130	ALA
2	f	198	LEU
2	f	256	PRO
2	i	130	ALA
2	g	198	LEU
2	g	256	PRO
2	j	130	ALA
4	y	62	GLU
4	U	60	GLU
4	V	60	GLU
4	V	79	MET
5	z	111	PRO
5	W	110	PRO
5	W	111	PRO
5	X	111	PRO
5	l	169	ARG
1	I	959	LEU
1	m	146	ASP
1	m	1283	LEU
1	o	766	PRO
2	2	255	ARG
2	3	131	VAL
2	3	271	VAL
2	e	255	ARG
2	h	131	VAL
2	h	271	VAL
2	f	255	ARG
2	i	131	VAL
2	i	271	VAL
2	g	255	ARG
2	j	131	VAL
2	j	271	VAL
4	y	61	VAL
4	S	61	VAL
4	S	62	GLU
4	V	61	VAL

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Mol	Chain	Res	Type
4	V	62	GLU
1	B	1334	TYR
1	C	1334	TYR
1	D	691	GLU
1	F	819	LEU
1	F	1322	LYS
1	k	985	THR
1	o	960	SER
1	p	960	SER
4	T	204	PRO
4	U	80	PRO
4	V	81	SER
5	X	309	TYR
1	B	930	PRO
1	C	986	LEU
1	F	148	LEU
1	F	821	ALA
1	F	960	SER
1	G	960	SER
1	H	1155	THR
1	H	1162	PRO
1	k	960	SER
1	m	960	SER
1	p	1335	GLY
2	2	67	GLU
2	3	129	ASP
2	h	129	ASP
2	i	129	ASP
2	j	129	ASP
4	S	60	GLU
5	Z	309	TYR
1	B	959	LEU
1	C	958	PRO
1	k	313	ALA
1	n	960	SER
1	o	765	GLU
4	y	60	GLU
5	z	101	GLU
5	b	129	VAL
1	E	959	LEU
1	I	960	SER
1	m	869	PRO

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Mol	Chain	Res	Type
1	p	1071	GLY
1	G	961	PRO
4	T	61	VAL
1	k	961	PRO
4	U	22	PRO
1	k	1298	PRO

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	1142/1156 (99%)	1128 (99%)	14 (1%)	67	79
1	B	1123/1156 (97%)	1110 (99%)	13 (1%)	67	79
1	C	1123/1156 (97%)	1105 (98%)	18 (2%)	58	74
1	D	1125/1156 (97%)	1108 (98%)	17 (2%)	60	75
1	E	1138/1156 (98%)	1131 (99%)	7 (1%)	84	88
1	F	1128/1156 (98%)	1112 (99%)	16 (1%)	62	76
1	G	1147/1156 (99%)	1134 (99%)	13 (1%)	70	80
1	H	1147/1156 (99%)	1132 (99%)	15 (1%)	65	77
1	I	1130/1156 (98%)	1119 (99%)	11 (1%)	73	82
1	k	1105/1156 (96%)	1091 (99%)	14 (1%)	65	77
1	l	1144/1156 (99%)	1129 (99%)	15 (1%)	65	77
1	m	1124/1156 (97%)	1105 (98%)	19 (2%)	56	72
1	n	1143/1156 (99%)	1130 (99%)	13 (1%)	70	80
1	o	1124/1156 (97%)	1111 (99%)	13 (1%)	67	79
1	p	1110/1156 (96%)	1101 (99%)	9 (1%)	79	85
1	q	1042/1156 (90%)	1031 (99%)	11 (1%)	70	80
2	2	159/596 (27%)	157 (99%)	2 (1%)	65	77
2	3	177/596 (30%)	174 (98%)	3 (2%)	56	72
2	e	159/596 (27%)	157 (99%)	2 (1%)	65	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f	159/596 (27%)	157 (99%)	2 (1%)	65	77
2	g	159/596 (27%)	157 (99%)	2 (1%)	65	77
2	h	177/596 (30%)	174 (98%)	3 (2%)	56	72
2	i	177/596 (30%)	174 (98%)	3 (2%)	56	72
2	j	177/596 (30%)	174 (98%)	3 (2%)	56	72
3	J	50/71 (70%)	49 (98%)	1 (2%)	50	68
3	K	49/71 (69%)	49 (100%)	0	100	100
3	L	49/71 (69%)	49 (100%)	0	100	100
3	M	49/71 (69%)	49 (100%)	0	100	100
3	N	49/71 (69%)	48 (98%)	1 (2%)	50	68
3	O	49/71 (69%)	49 (100%)	0	100	100
3	P	49/71 (69%)	48 (98%)	1 (2%)	50	68
3	Q	49/71 (69%)	49 (100%)	0	100	100
3	R	49/71 (69%)	49 (100%)	0	100	100
3	r	50/71 (70%)	48 (96%)	2 (4%)	27	48
3	s	49/71 (69%)	48 (98%)	1 (2%)	50	68
3	t	49/71 (69%)	47 (96%)	2 (4%)	26	47
3	u	50/71 (70%)	49 (98%)	1 (2%)	50	68
3	v	50/71 (70%)	49 (98%)	1 (2%)	50	68
3	w	50/71 (70%)	49 (98%)	1 (2%)	50	68
3	x	48/71 (68%)	48 (100%)	0	100	100
4	S	251/255 (98%)	251 (100%)	0	100	100
4	T	251/255 (98%)	251 (100%)	0	100	100
4	U	251/255 (98%)	247 (98%)	4 (2%)	58	74
4	V	251/255 (98%)	248 (99%)	3 (1%)	67	79
4	y	216/255 (85%)	214 (99%)	2 (1%)	75	83
5	1	229/275 (83%)	228 (100%)	1 (0%)	89	91
5	W	253/275 (92%)	250 (99%)	3 (1%)	67	79
5	X	249/275 (90%)	246 (99%)	3 (1%)	67	79
5	Y	254/275 (92%)	253 (100%)	1 (0%)	89	91
5	Z	253/275 (92%)	249 (98%)	4 (2%)	58	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	a	238/275 (86%)	234 (98%)	4 (2%)	56	72
5	b	241/275 (88%)	237 (98%)	4 (2%)	56	72
5	c	245/275 (89%)	243 (99%)	2 (1%)	79	85
5	d	245/275 (89%)	243 (99%)	2 (1%)	79	85
5	z	256/275 (93%)	250 (98%)	6 (2%)	45	64
All	All	23810/28425 (84%)	23522 (99%)	288 (1%)	66	79

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	312	ASN
1	A	436	ARG
1	A	748	ARG
1	A	757	ARG
1	A	772	ARG
1	A	773	ARG
1	A	787	LEU
1	A	788	CYS
1	A	1019	THR
1	A	1064	ASN
1	A	1093	ARG
1	A	1153	ARG
1	A	1297	LYS
1	B	37	ARG
1	B	148	LEU
1	B	168	THR
1	B	198	MET
1	B	312	ASN
1	B	436	ARG
1	B	662	ARG
1	B	773	ARG
1	B	1019	THR
1	B	1061	VAL
1	B	1064	ASN
1	B	1093	ARG
1	B	1297	LYS
1	C	51	PHE
1	C	128	ILE
1	C	148	LEU

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Mol	Chain	Res	Type
1	C	198	MET
1	C	312	ASN
1	C	358	MET
1	C	363	VAL
1	C	374	ARG
1	C	436	ARG
1	C	662	ARG
1	C	663	LEU
1	C	748	ARG
1	C	772	ARG
1	C	773	ARG
1	C	1019	THR
1	C	1064	ASN
1	C	1093	ARG
1	C	1297	LYS
1	D	128	ILE
1	D	198	MET
1	D	312	ASN
1	D	436	ARG
1	D	618	LEU
1	D	662	ARG
1	D	663	LEU
1	D	691	GLU
1	D	692	LEU
1	D	748	ARG
1	D	757	ARG
1	D	773	ARG
1	D	1019	THR
1	D	1064	ASN
1	D	1153	ARG
1	D	1297	LYS
1	D	1321	LEU
1	E	312	ASN
1	E	748	ARG
1	E	772	ARG
1	E	773	ARG
1	E	1032	LEU
1	E	1093	ARG
1	E	1297	LYS
1	F	37	ARG
1	F	123	LYS
1	F	148	LEU

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Mol	Chain	Res	Type
1	F	198	MET
1	F	235	ARG
1	F	312	ASN
1	F	436	ARG
1	F	748	ARG
1	F	757	ARG
1	F	772	ARG
1	F	773	ARG
1	F	1019	THR
1	F	1064	ASN
1	F	1160	LEU
1	F	1297	LYS
1	F	1321	LEU
1	G	37	ARG
1	G	128	ILE
1	G	198	MET
1	G	312	ASN
1	G	363	VAL
1	G	662	ARG
1	G	748	ARG
1	G	772	ARG
1	G	773	ARG
1	G	834	THR
1	G	1064	ASN
1	G	1171	ARG
1	G	1297	LYS
1	H	37	ARG
1	H	198	MET
1	H	312	ASN
1	H	436	ARG
1	H	646	LEU
1	H	662	ARG
1	H	772	ARG
1	H	773	ARG
1	H	842	LEU
1	H	1018	LEU
1	H	1021	VAL
1	H	1064	ASN
1	H	1093	ARG
1	H	1297	LYS
1	H	1331	GLU
1	I	198	MET

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Mol	Chain	Res	Type
1	I	312	ASN
1	I	662	ARG
1	I	748	ARG
1	I	772	ARG
1	I	773	ARG
1	I	959	LEU
1	I	1019	THR
1	I	1064	ASN
1	I	1093	ARG
1	I	1297	LYS
1	k	37	ARG
1	k	198	MET
1	k	207	MET
1	k	302	SER
1	k	662	ARG
1	k	748	ARG
1	k	772	ARG
1	k	773	ARG
1	k	788	CYS
1	k	1019	THR
1	k	1064	ASN
1	k	1093	ARG
1	k	1160	LEU
1	k	1297	LYS
1	l	37	ARG
1	l	128	ILE
1	l	312	ASN
1	l	436	ARG
1	l	644	ARG
1	l	662	ARG
1	l	698	ARG
1	l	748	ARG
1	l	772	ARG
1	l	773	ARG
1	l	1064	ASN
1	l	1093	ARG
1	l	1143	LYS
1	l	1239	ASN
1	l	1297	LYS
1	m	51	PHE
1	m	117	VAL
1	m	147	THR

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Mol	Chain	Res	Type
1	m	312	ASN
1	m	436	ARG
1	m	517	ASP
1	m	647	LEU
1	m	662	ARG
1	m	663	LEU
1	m	748	ARG
1	m	757	ARG
1	m	772	ARG
1	m	773	ARG
1	m	842	LEU
1	m	844	ARG
1	m	1032	LEU
1	m	1064	ASN
1	m	1093	ARG
1	m	1297	LYS
1	n	37	ARG
1	n	312	ASN
1	n	436	ARG
1	n	575	LEU
1	n	691	GLU
1	n	748	ARG
1	n	772	ARG
1	n	773	ARG
1	n	998	LYS
1	n	1019	THR
1	n	1064	ASN
1	n	1297	LYS
1	n	1332	THR
1	o	37	ARG
1	o	312	ASN
1	o	487	ARG
1	o	488	GLU
1	o	748	ARG
1	o	765	GLU
1	o	772	ARG
1	o	773	ARG
1	o	972	ARG
1	o	1064	ASN
1	o	1093	ARG
1	o	1297	LYS
1	o	1298	PRO

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Mol	Chain	Res	Type
1	p	312	ASN
1	p	734	VAL
1	p	757	ARG
1	p	772	ARG
1	p	773	ARG
1	p	1019	THR
1	p	1064	ASN
1	p	1093	ARG
1	p	1297	LYS
1	q	269	ARG
1	q	305	LYS
1	q	358	MET
1	q	373	LEU
1	q	423	ASN
1	q	851	ASN
1	q	852	VAL
1	q	972	ARG
1	q	1010	MET
1	q	1122	ARG
1	q	1220	ARG
2	2	202	ASP
2	2	295	ARG
2	3	94	LEU
2	3	272	ASP
2	3	295	ARG
2	e	202	ASP
2	e	295	ARG
2	h	94	LEU
2	h	272	ASP
2	h	295	ARG
2	f	202	ASP
2	f	295	ARG
2	i	94	LEU
2	i	272	ASP
2	i	295	ARG
2	g	202	ASP
2	g	295	ARG
2	j	94	LEU
2	j	272	ASP
2	j	295	ARG
3	J	85	LEU
3	N	85	LEU

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Mol	Chain	Res	Type
3	P	85	LEU
3	r	60	VAL
3	r	85	LEU
3	s	85	LEU
3	t	85	LEU
3	t	87	MET
3	u	85	LEU
3	v	85	LEU
3	w	85	LEU
4	y	75	THR
4	y	226	ARG
4	U	60	GLU
4	U	160	LEU
4	U	203	ARG
4	U	209	VAL
4	V	6	SER
4	V	79	MET
4	V	160	LEU
5	z	23	ARG
5	z	45	LEU
5	z	54	ARG
5	z	74	VAL
5	z	102	LYS
5	z	308	ILE
5	W	54	ARG
5	W	109	LEU
5	W	169	ARG
5	X	21	LEU
5	X	54	ARG
5	X	308	ILE
5	Y	54	ARG
5	Z	13	LEU
5	Z	54	ARG
5	Z	102	LYS
5	Z	308	ILE
5	1	143	ASN
5	a	45	LEU
5	a	51	ASP
5	a	143	ASN
5	a	169	ARG
5	b	45	LEU
5	b	128	LEU

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Mol	Chain	Res	Type
5	b	129	VAL
5	b	143	ASN
5	c	45	LEU
5	c	143	ASN
5	d	143	ASN
5	d	169	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (406) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	77	HIS
1	A	282	GLN
1	A	312	ASN
1	A	439	GLN
1	A	536	HIS
1	A	562	ASN
1	A	639	ASN
1	A	675	HIS
1	A	712	HIS
1	A	863	HIS
1	A	867	HIS
1	A	984	HIS
1	A	1060	HIS
1	A	1064	ASN
1	A	1095	GLN
1	A	1104	HIS
1	A	1207	GLN
1	A	1274	GLN
1	B	23	HIS
1	B	77	HIS
1	B	97	GLN
1	B	159	ASN
1	B	218	GLN
1	B	286	ASN
1	B	312	ASN
1	B	328	GLN
1	B	338	GLN
1	B	372	HIS
1	B	439	GLN
1	B	443	HIS
1	B	492	HIS

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Mol	Chain	Res	Type
1	B	597	GLN
1	B	606	HIS
1	B	620	HIS
1	B	795	ASN
1	B	903	ASN
1	B	996	HIS
1	B	1013	HIS
1	B	1063	GLN
1	B	1064	ASN
1	B	1095	GLN
1	B	1175	ASN
1	B	1207	GLN
1	B	1248	GLN
1	B	1257	ASN
1	C	23	HIS
1	C	82	HIS
1	C	159	ASN
1	C	200	HIS
1	C	239	GLN
1	C	282	GLN
1	C	312	ASN
1	C	345	GLN
1	C	372	HIS
1	C	439	GLN
1	C	592	HIS
1	C	675	HIS
1	C	712	HIS
1	C	795	ASN
1	C	836	ASN
1	C	863	HIS
1	C	899	HIS
1	C	969	HIS
1	C	996	HIS
1	C	1060	HIS
1	C	1064	ASN
1	C	1257	ASN
1	C	1336	ASN
1	C	1347	GLN
1	D	159	ASN
1	D	312	ASN
1	D	439	GLN
1	D	492	HIS

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Mol	Chain	Res	Type
1	D	675	HIS
1	D	836	ASN
1	D	863	HIS
1	D	887	HIS
1	D	898	GLN
1	D	899	HIS
1	D	996	HIS
1	D	1082	HIS
1	D	1095	GLN
1	D	1257	ASN
1	D	1309	HIS
1	D	1320	GLN
1	E	82	HIS
1	E	200	HIS
1	E	282	GLN
1	E	312	ASN
1	E	328	GLN
1	E	349	GLN
1	E	372	HIS
1	E	379	ASN
1	E	413	ASN
1	E	439	GLN
1	E	492	HIS
1	E	607	GLN
1	E	639	ASN
1	E	675	HIS
1	E	763	GLN
1	E	797	HIS
1	E	836	ASN
1	E	863	HIS
1	E	899	HIS
1	E	937	ASN
1	E	1060	HIS
1	E	1063	GLN
1	E	1099	GLN
1	E	1259	ASN
1	E	1274	GLN
1	E	1352	ASN
1	F	23	HIS
1	F	77	HIS
1	F	139	HIS
1	F	159	ASN

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Mol	Chain	Res	Type
1	F	282	GLN
1	F	286	ASN
1	F	312	ASN
1	F	439	GLN
1	F	492	HIS
1	F	620	HIS
1	F	643	GLN
1	F	797	HIS
1	F	835	ASN
1	F	863	HIS
1	F	898	GLN
1	F	899	HIS
1	F	915	GLN
1	F	969	HIS
1	F	1064	ASN
1	F	1095	GLN
1	F	1274	GLN
1	F	1347	GLN
1	F	1352	ASN
1	G	159	ASN
1	G	282	GLN
1	G	312	ASN
1	G	319	HIS
1	G	372	HIS
1	G	639	ASN
1	G	678	ASN
1	G	722	GLN
1	G	863	HIS
1	G	867	HIS
1	G	873	GLN
1	G	937	ASN
1	G	997	HIS
1	G	1099	GLN
1	G	1257	ASN
1	G	1336	ASN
1	G	1347	GLN
1	H	82	HIS
1	H	159	ASN
1	H	312	ASN
1	H	328	GLN
1	H	338	GLN
1	H	439	GLN

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Mol	Chain	Res	Type
1	H	443	HIS
1	H	492	HIS
1	H	863	HIS
1	H	898	GLN
1	H	899	HIS
1	H	951	GLN
1	H	969	HIS
1	H	996	HIS
1	H	1063	GLN
1	H	1064	ASN
1	H	1095	GLN
1	H	1099	GLN
1	H	1257	ASN
1	H	1259	ASN
1	H	1274	GLN
1	H	1347	GLN
1	I	82	HIS
1	I	312	ASN
1	I	439	GLN
1	I	492	HIS
1	I	675	HIS
1	I	836	ASN
1	I	863	HIS
1	I	899	HIS
1	I	996	HIS
1	I	1060	HIS
1	I	1064	ASN
1	I	1066	ASN
1	I	1207	GLN
1	I	1219	GLN
1	k	77	HIS
1	k	82	HIS
1	k	97	GLN
1	k	159	ASN
1	k	372	HIS
1	k	439	GLN
1	k	675	HIS
1	k	712	HIS
1	k	795	ASN
1	k	863	HIS
1	k	898	GLN
1	k	899	HIS

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Mol	Chain	Res	Type
1	k	951	GLN
1	k	984	HIS
1	k	996	HIS
1	k	1060	HIS
1	k	1064	ASN
1	k	1082	HIS
1	k	1239	ASN
1	k	1320	GLN
1	l	23	HIS
1	l	159	ASN
1	l	286	ASN
1	l	312	ASN
1	l	328	GLN
1	l	338	GLN
1	l	372	HIS
1	l	433	ASN
1	l	439	GLN
1	l	492	HIS
1	l	675	HIS
1	l	749	ASN
1	l	795	ASN
1	l	863	HIS
1	l	899	HIS
1	l	937	ASN
1	l	951	GLN
1	l	1064	ASN
1	l	1082	HIS
1	l	1239	ASN
1	l	1259	ASN
1	l	1274	GLN
1	l	1303	GLN
1	l	1333	HIS
1	l	1352	ASN
1	m	4	ASN
1	m	23	HIS
1	m	112	GLN
1	m	282	GLN
1	m	286	ASN
1	m	312	ASN
1	m	328	GLN
1	m	372	HIS
1	m	443	HIS

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Mol	Chain	Res	Type
1	m	492	HIS
1	m	592	HIS
1	m	639	ASN
1	m	675	HIS
1	m	835	ASN
1	m	836	ASN
1	m	863	HIS
1	m	898	GLN
1	m	899	HIS
1	m	937	ASN
1	m	969	HIS
1	m	996	HIS
1	m	1013	HIS
1	m	1060	HIS
1	m	1063	GLN
1	m	1064	ASN
1	m	1082	HIS
1	m	1274	GLN
1	m	1303	GLN
1	n	23	HIS
1	n	112	GLN
1	n	159	ASN
1	n	312	ASN
1	n	319	HIS
1	n	492	HIS
1	n	712	HIS
1	n	797	HIS
1	n	863	HIS
1	n	898	GLN
1	n	899	HIS
1	n	903	ASN
1	n	951	GLN
1	n	969	HIS
1	n	971	HIS
1	n	996	HIS
1	n	1060	HIS
1	n	1064	ASN
1	n	1095	GLN
1	n	1099	GLN
1	n	1248	GLN
1	n	1259	ASN
1	n	1314	GLN

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Mol	Chain	Res	Type
1	n	1352	ASN
1	o	23	HIS
1	o	77	HIS
1	o	112	GLN
1	o	282	GLN
1	o	312	ASN
1	o	345	GLN
1	o	349	GLN
1	o	372	HIS
1	o	413	ASN
1	o	439	GLN
1	o	579	GLN
1	o	639	ASN
1	o	675	HIS
1	o	722	GLN
1	o	863	HIS
1	o	969	HIS
1	o	996	HIS
1	o	997	HIS
1	o	1064	ASN
1	o	1104	HIS
1	o	1274	GLN
1	o	1303	GLN
1	p	139	HIS
1	p	159	ASN
1	p	167	ASN
1	p	212	GLN
1	p	218	GLN
1	p	282	GLN
1	p	286	ASN
1	p	312	ASN
1	p	492	HIS
1	p	512	ASN
1	p	696	ASN
1	p	863	HIS
1	p	899	HIS
1	p	951	GLN
1	p	1063	GLN
1	p	1064	ASN
1	p	1066	ASN
1	p	1082	HIS
1	p	1095	GLN

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Mol	Chain	Res	Type
1	p	1104	HIS
1	p	1152	GLN
1	p	1257	ASN
1	p	1259	ASN
1	p	1274	GLN
1	q	77	HIS
1	q	154	ASN
1	q	423	ASN
1	q	424	GLN
1	q	433	ASN
1	q	443	HIS
1	q	472	GLN
1	q	639	ASN
1	q	675	HIS
1	q	796	ASN
1	q	851	ASN
1	q	863	HIS
1	q	887	HIS
1	q	945	ASN
1	q	1248	GLN
1	q	1292	ASN
1	q	1320	GLN
2	3	91	HIS
2	3	184	ASN
2	3	265	ASN
2	h	91	HIS
2	h	184	ASN
2	h	265	ASN
2	i	69	GLN
2	i	91	HIS
2	i	184	ASN
2	i	265	ASN
2	j	91	HIS
2	j	184	ASN
2	j	265	ASN
3	J	43	GLN
3	J	58	GLN
3	K	58	GLN
3	M	58	GLN
3	R	58	GLN
3	r	50	ASN
3	v	81	GLN

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Mol	Chain	Res	Type
3	x	50	ASN
4	y	215	HIS
4	y	233	HIS
4	y	237	ASN
4	S	96	ASN
4	S	155	HIS
4	S	197	ASN
4	S	217	HIS
4	T	215	HIS
4	T	221	ASN
4	U	215	HIS
4	U	237	ASN
4	V	45	HIS
4	V	155	HIS
4	V	215	HIS
4	V	237	ASN
5	z	78	GLN
5	z	231	GLN
5	z	290	GLN
5	W	94	ASN
5	W	158	HIS
5	X	231	GLN
5	X	290	GLN
5	Y	88	GLN
5	Y	205	ASN
5	Y	231	GLN
5	l	11	GLN
5	a	11	GLN
5	a	86	HIS
5	a	143	ASN
5	a	144	GLN
5	b	78	GLN
5	b	143	ASN
5	c	11	GLN
5	c	144	GLN
5	d	11	GLN
5	d	143	ASN
5	d	144	GLN

5.3.3 RNA ⓘ

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.

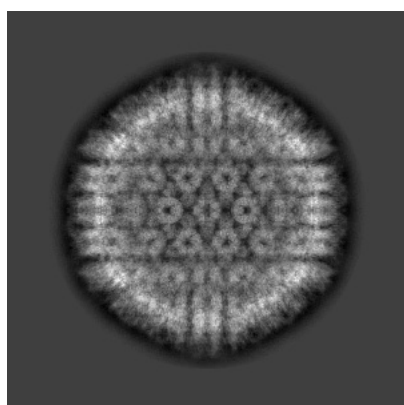
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9366. These allow visual inspection of the internal detail of the map and identification of artifacts.

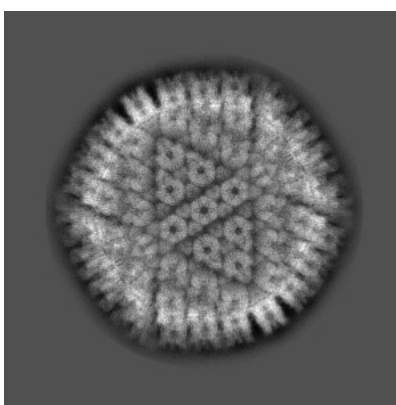
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

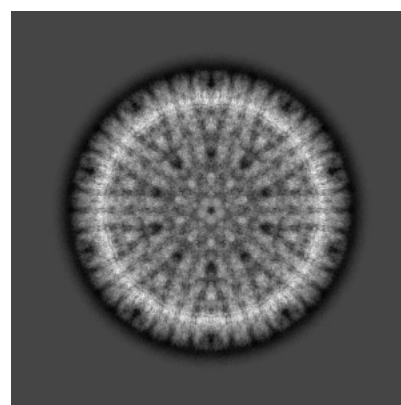
6.1.1 Primary map



X



Y

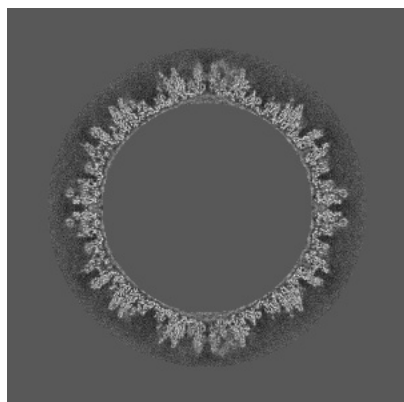


Z

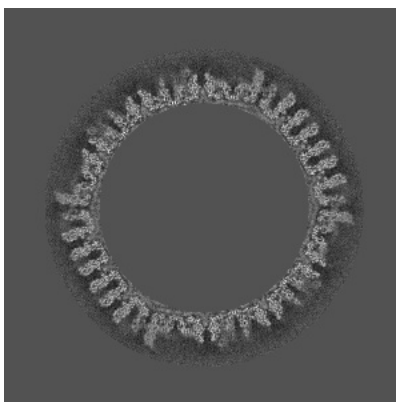
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

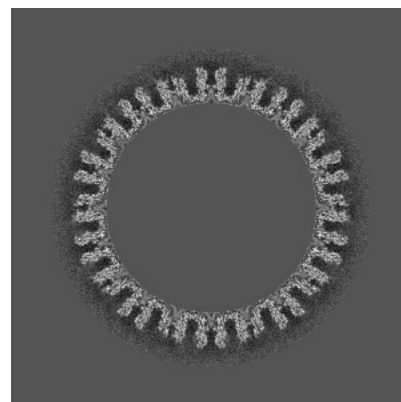
6.2.1 Primary map



X Index: 640



Y Index: 640

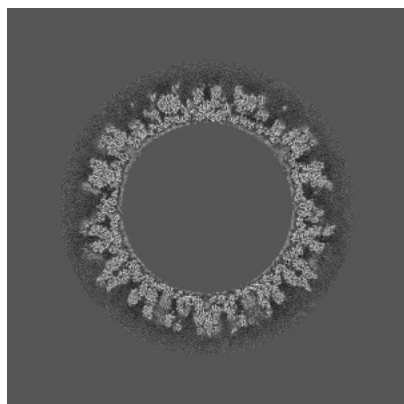


Z Index: 640

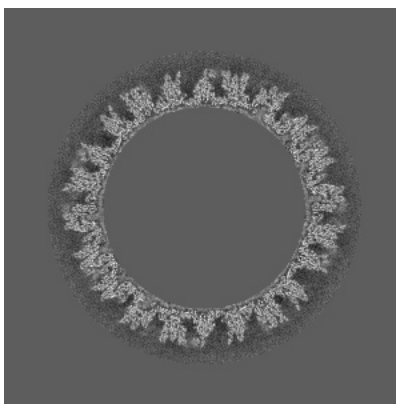
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

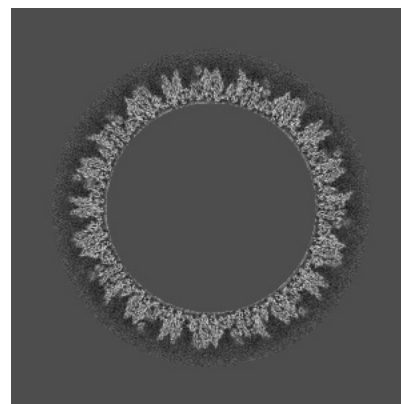
6.3.1 Primary map



X Index: 445



Y Index: 731

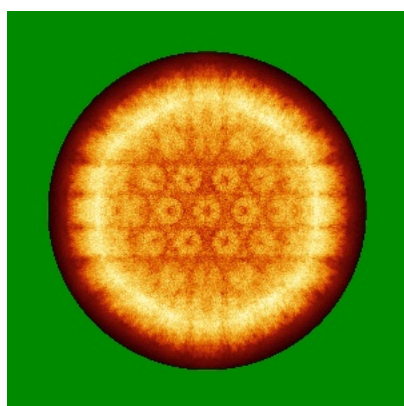


Z Index: 618

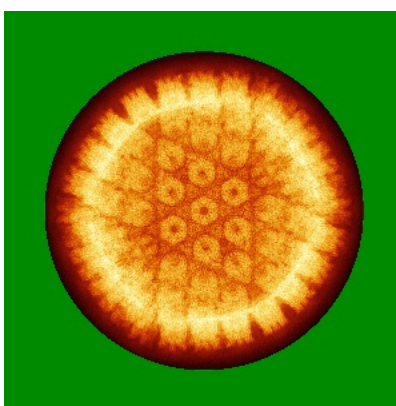
The images above show the largest variance slices of the map in three orthogonal directions.

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

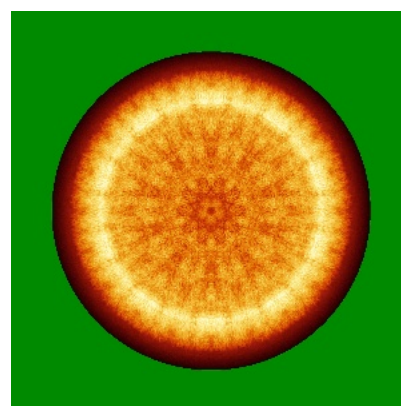
6.4.1 Primary map



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 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

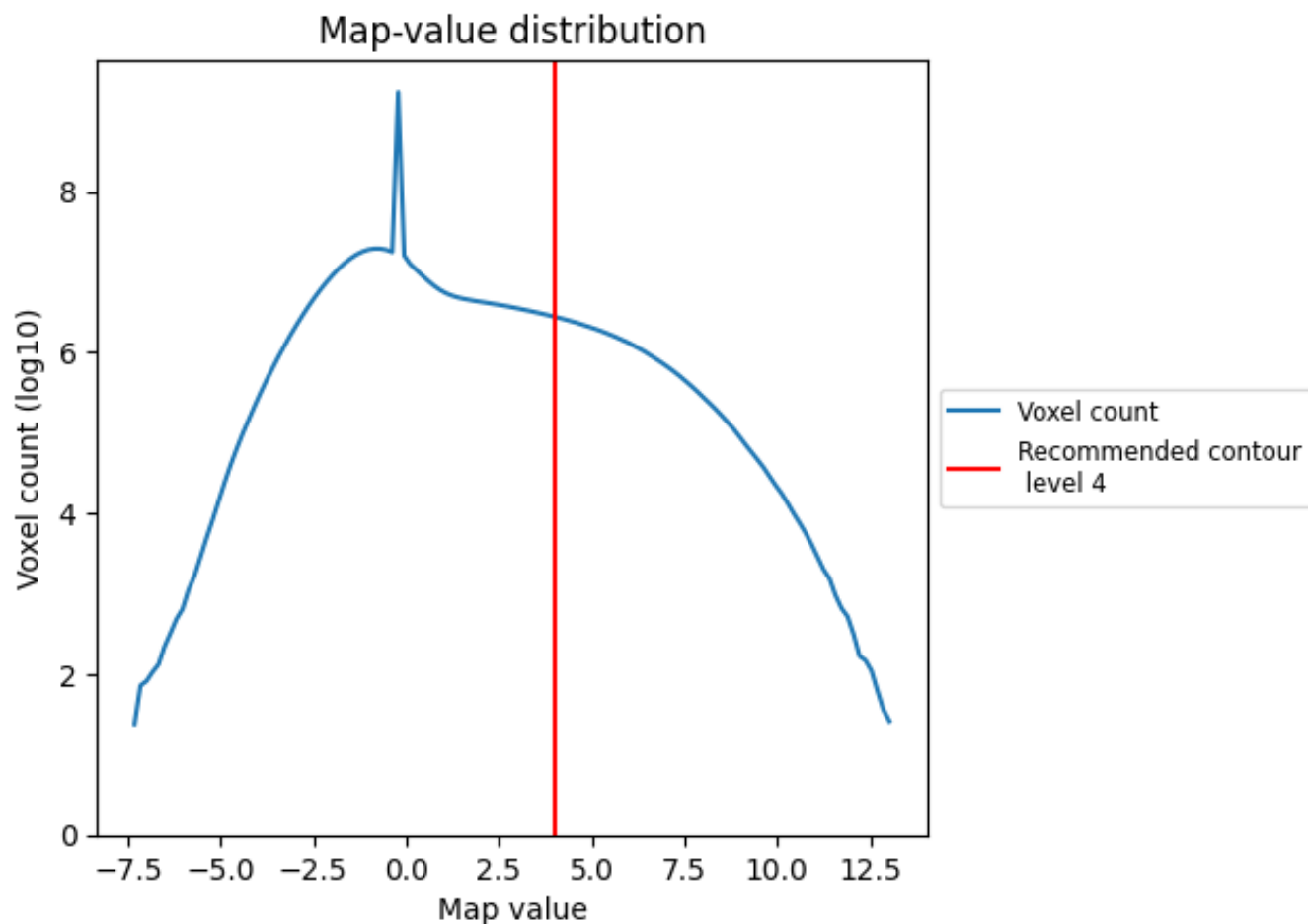
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

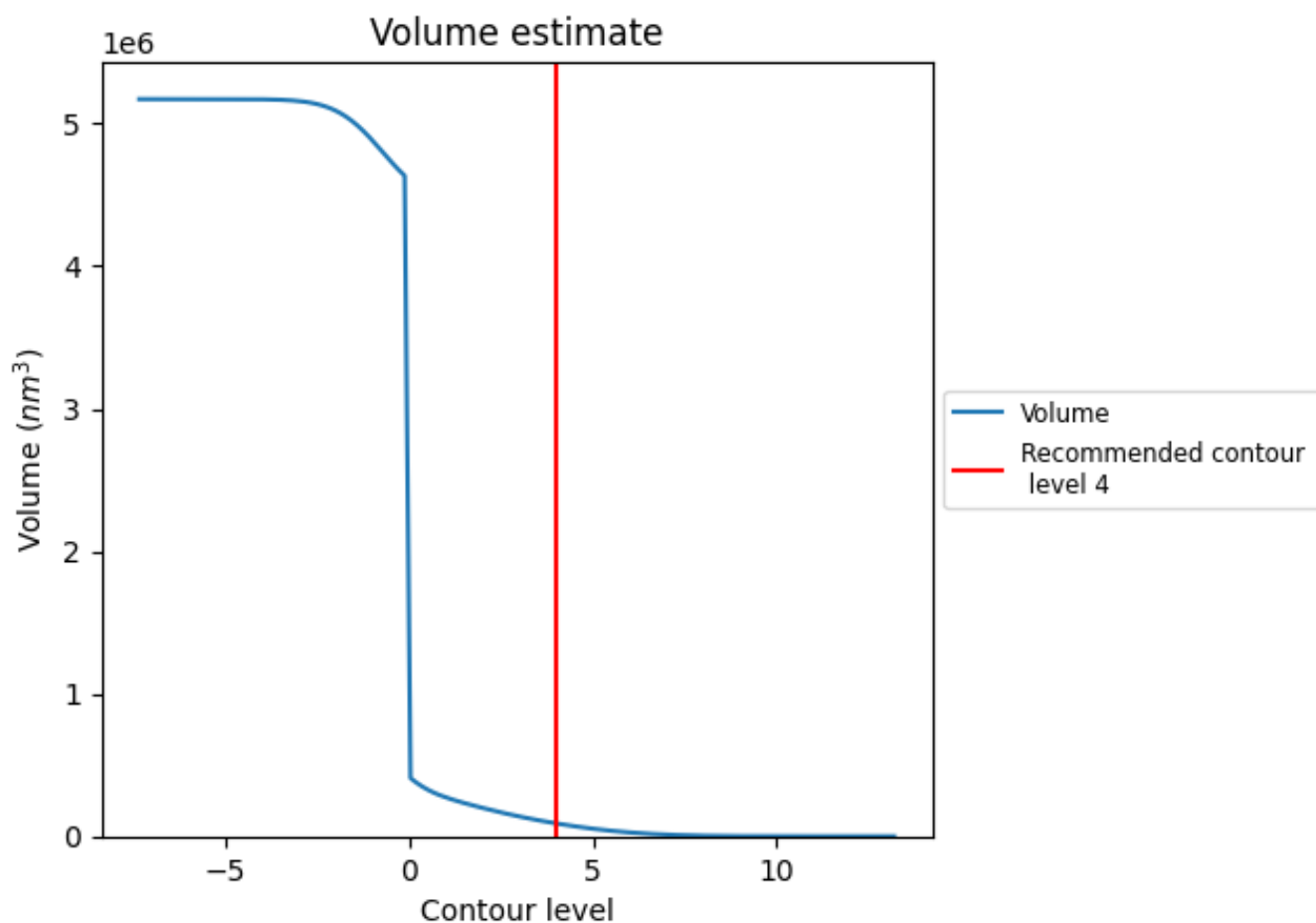
This section contains the results of statistical analysis of the map.

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.

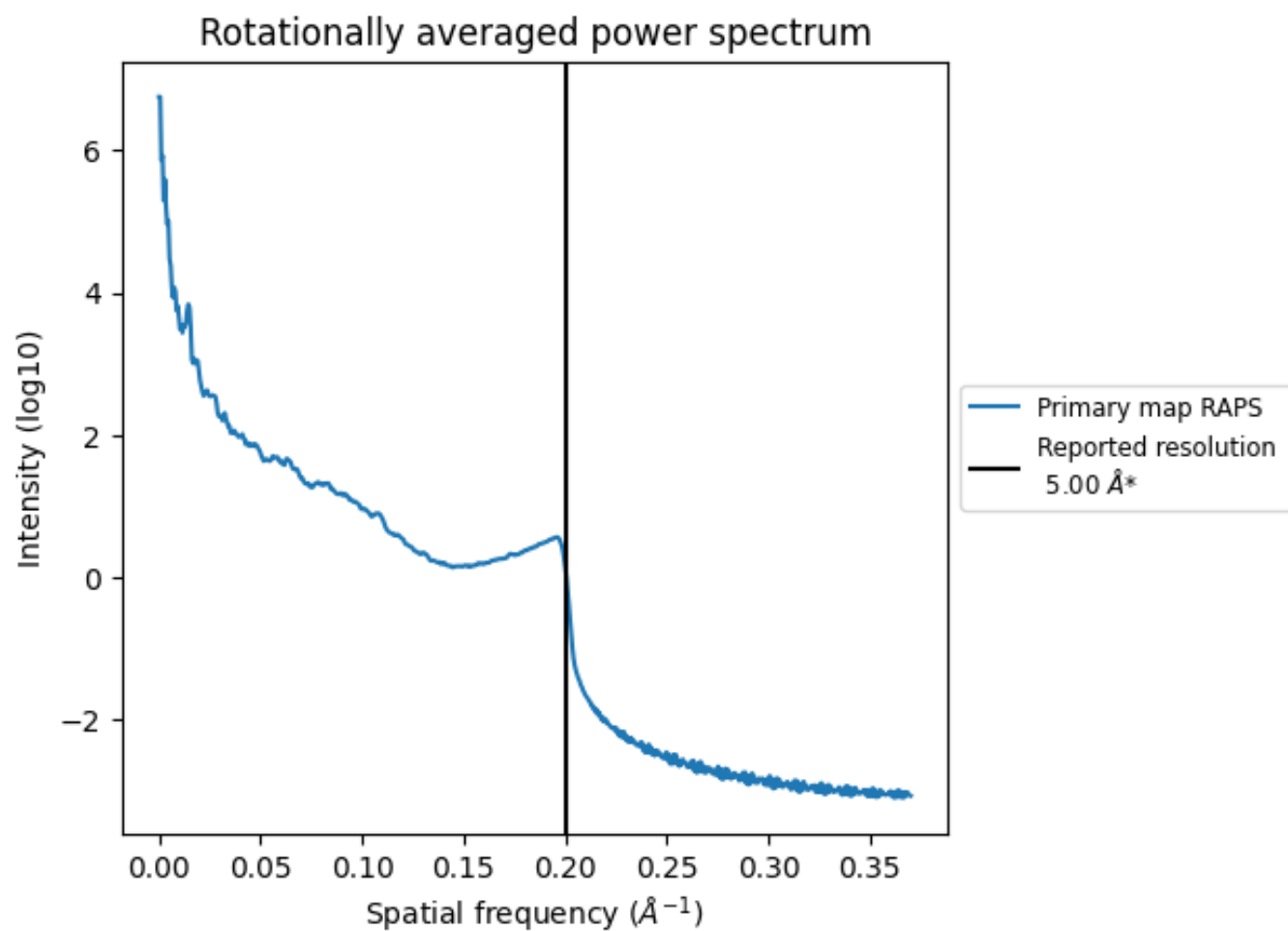
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90561 nm³; this corresponds to an approximate mass of 81806 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 0.200 Å⁻¹

8 Fourier-Shell correlation ⓘ

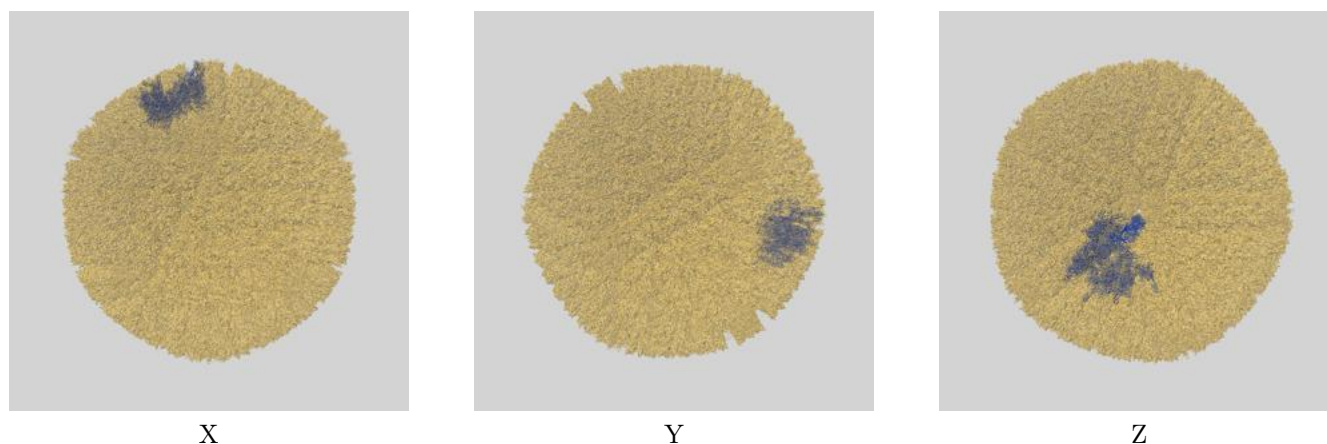
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

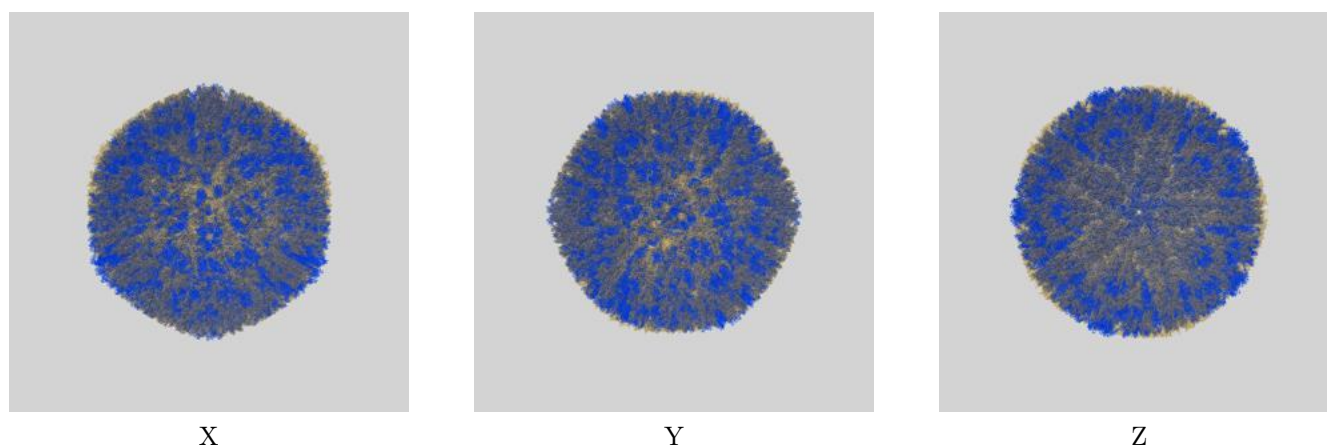
This section contains information regarding the fit between EMDB map EMD-9366 and PDB model 6NHJ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

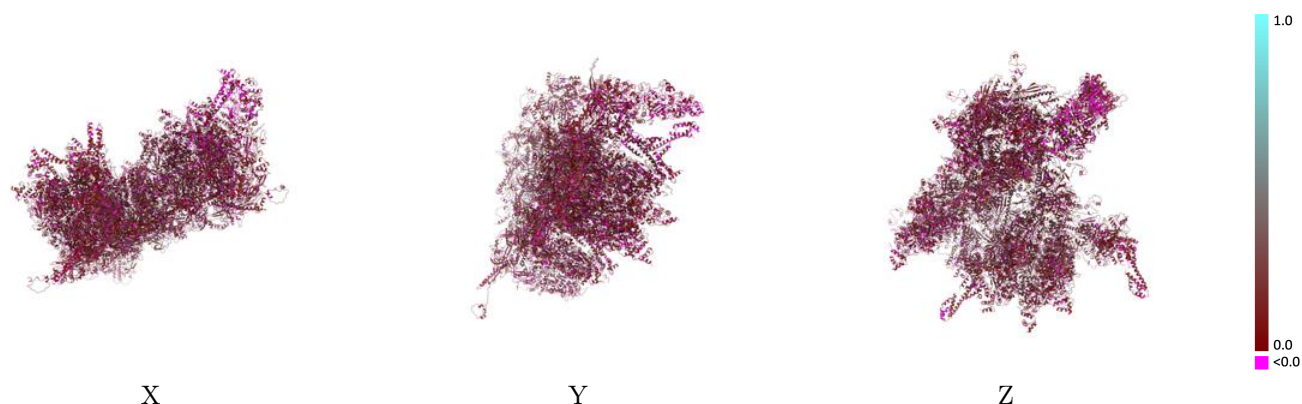


9.1.2 Map-model assembly overlay [i](#)



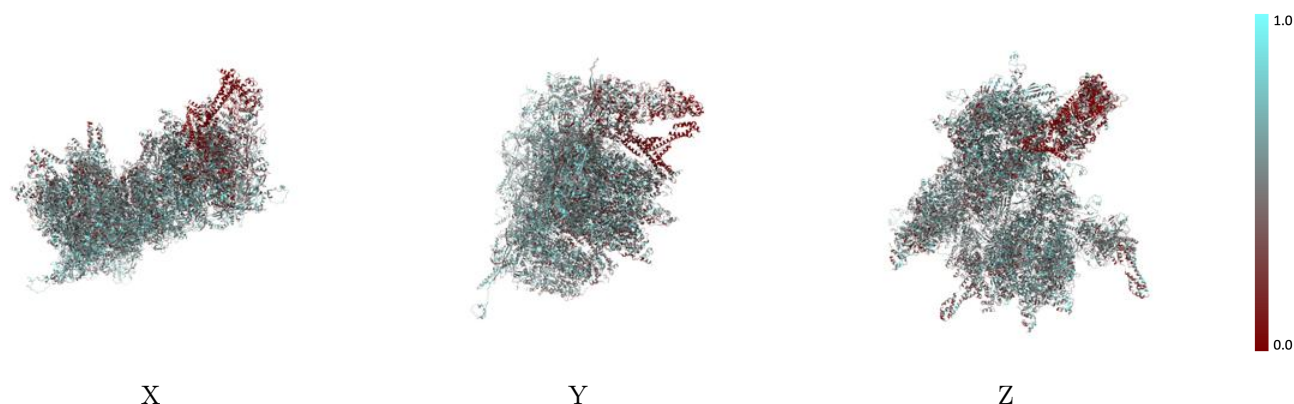
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



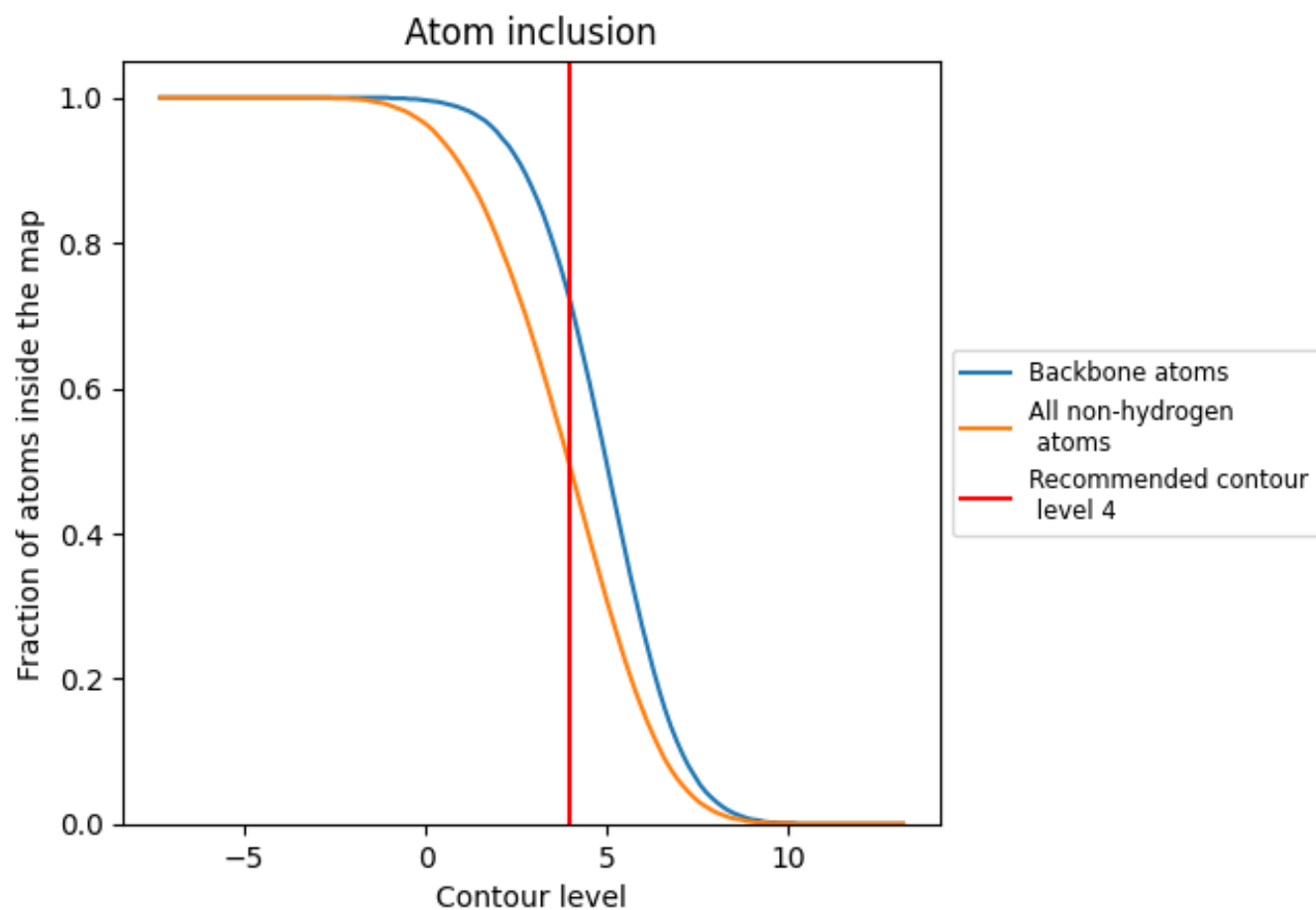
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 49% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4900	 0.1390
1	 0.2890	 0.1150
2	 0.0080	 0.0720
3	 0.0220	 0.0940
A	 0.5450	 0.1570
B	 0.5470	 0.1490
C	 0.5370	 0.1410
D	 0.5280	 0.1390
E	 0.5370	 0.1490
F	 0.5400	 0.1530
G	 0.5260	 0.1470
H	 0.5170	 0.1340
I	 0.5190	 0.1270
J	 0.4730	 0.1410
K	 0.4540	 0.1350
L	 0.4360	 0.1300
M	 0.4120	 0.1250
N	 0.4520	 0.1270
O	 0.4340	 0.1210
P	 0.4470	 0.1160
Q	 0.4540	 0.1730
R	 0.4410	 0.0880
S	 0.4790	 0.1310
T	 0.4810	 0.1380
U	 0.5040	 0.1500
V	 0.4940	 0.1260
W	 0.4890	 0.1610
X	 0.4740	 0.1550
Y	 0.4990	 0.1580
Z	 0.4640	 0.1350
a	 0.4880	 0.1430
b	 0.4740	 0.1530
c	 0.4670	 0.1350
d	 0.4430	 0.1250
e	 0.4230	 0.1290



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Chain	Atom inclusion	Q-score
f	 0.3670	 0.1160
g	 0.3650	 0.1090
h	 0.4260	 0.1230
i	 0.4090	 0.1310
j	 0.4000	 0.1230
k	 0.5010	 0.1470
l	 0.5270	 0.1480
m	 0.5250	 0.1390
n	 0.5140	 0.1360
o	 0.5220	 0.1370
p	 0.5090	 0.1490
q	 0.3280	 0.1180
r	 0.4080	 0.1110
s	 0.4340	 0.1440
t	 0.4340	 0.1220
u	 0.3970	 0.1250
v	 0.4470	 0.1270
w	 0.4170	 0.1250
x	 0.0570	 0.0410
y	 0.3460	 0.1190
z	 0.3360	 0.1290