



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 10:26 PM EDT

PDB ID : 5VKU
EMDB ID : EMD-8703
Title : An atomic structure of the human cytomegalovirus (HCMV) capsid with its securing layer of pp150 tegument protein
Authors : Yu, X.; Jih, J.; Jiang, J.; Zhou, H.
Deposited on : 2017-04-24
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

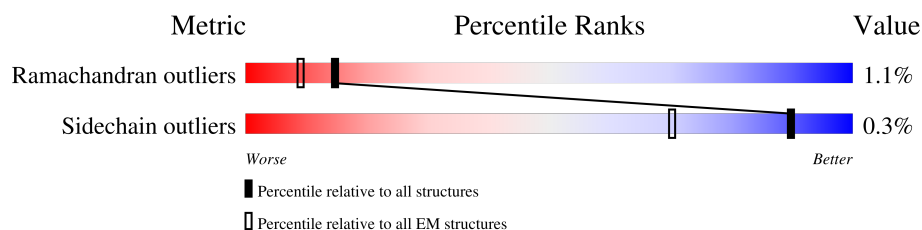
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	0	285	<div> <div>58%</div> <div>99%</div> </div>
1	1	285	<div> <div>56%</div> <div>99%</div> </div>
1	2	285	<div> <div>93%</div> <div>99%</div> </div>
1	3	285	<div> <div>75%</div> <div>98%</div> </div>
1	4	285	<div> <div>53%</div> <div>99%</div> </div>
1	5	285	<div> <div>63%</div> <div>99%</div> </div>
1	6	285	<div> <div>60%</div> <div>99%</div> </div>
1	7	285	<div> <div>49%</div> <div>99%</div> </div>
1	8	285	<div> <div>59%</div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
1	9	285	60% 99% 97%
1	v	285	97% 97%
1	w	285	99% 99%
1	x	285	85% 98%
1	y	285	54% 99%
1	z	285	53% 99%
2	A	1370	68% 96% ..
2	B	1370	46% 95% ..
2	C	1370	39% 97% ..
2	D	1370	36% 97% ..
2	E	1370	34% 96% ..
2	F	1370	38% 97% ..
2	G	1370	47% 97% ..
2	H	1370	31% 98% ..
2	I	1370	30% 97% ..
2	J	1370	29% 96% ..
2	K	1370	29% 98% ..
2	L	1370	30% 98% ..
2	M	1370	34% 98% ..
2	N	1370	30% 98% ..
2	O	1370	29% 97% ..
2	P	1370	31% 97% ..
3	Q	75	68% 84% 16%
3	R	75	67% 84% 16%
3	S	75	56% 84% 16%

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Mol	Chain	Length	Quality of chain
3	T	75	<div> <div>55%</div> <div>84%</div> <div>16%</div> </div>
3	U	75	<div> <div>56%</div> <div>84%</div> <div>16%</div> </div>
3	V	75	<div> <div>57%</div> <div>83%</div> <div>16%</div> </div>
3	W	75	<div> <div>64%</div> <div>84%</div> <div>16%</div> </div>
3	X	75	<div> <div>52%</div> <div>84%</div> <div>16%</div> </div>
3	Y	75	<div> <div>47%</div> <div>83%</div> <div>16%</div> </div>
3	Z	75	<div> <div>43%</div> <div>84%</div> <div>16%</div> </div>
3	a	75	<div> <div>51%</div> <div>84%</div> <div>16%</div> </div>
3	b	75	<div> <div>49%</div> <div>83%</div> <div>16%</div> </div>
3	c	75	<div> <div>53%</div> <div>84%</div> <div>16%</div> </div>
3	d	75	<div> <div>41%</div> <div>84%</div> <div>16%</div> </div>
3	e	75	<div> <div>40%</div> <div>84%</div> <div>16%</div> </div>
3	f	75	<div> <div>45%</div> <div>84%</div> <div>16%</div> </div>
4	g	290	<div> <div>74%</div> <div>88%</div> <div>10%</div> </div>
4	j	290	<div> <div>30%</div> <div>98%</div> <div>.</div> </div>
4	m	290	<div> <div>39%</div> <div>99%</div> <div>.</div> </div>
4	p	290	<div> <div>32%</div> <div>98%</div> <div>.</div> </div>
4	s	290	<div> <div>29%</div> <div>98%</div> <div>.</div> </div>
5	h	306	<div> <div>69%</div> <div>92%</div> <div>5%</div> </div>
5	i	306	<div> <div>76%</div> <div>92%</div> <div>7%</div> </div>
5	k	306	<div> <div>34%</div> <div>93%</div> <div>5%</div> </div>
5	l	306	<div> <div>36%</div> <div>98%</div> <div>..</div> </div>
5	n	306	<div> <div>41%</div> <div>94%</div> <div>.</div> </div>
5	o	306	<div> <div>39%</div> <div>94%</div> <div>5%</div> </div>
5	q	306	<div> <div>33%</div> <div>96%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	r	306	<div><div>32%</div><div>97%</div><div>..</div></div>
5	t	306	<div><div>31%</div><div>95%</div><div>..</div></div>
5	u	306	<div><div>34%</div><div>98%</div><div>..</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 248627 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 Tegument protein pp150.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	1	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	2	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	3	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	4	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	5	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	6	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	7	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	8	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	9	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	v	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	w	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	x	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	y	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	z	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1329	Total	C	N	O	S	0	0
			10527	6711	1822	1933	61		
2	B	1335	Total	C	N	O	S	0	0
			10574	6733	1830	1950	61		
2	C	1349	Total	C	N	O	S	0	0
			10686	6805	1852	1968	61		
2	D	1346	Total	C	N	O	S	0	0
			10670	6796	1849	1964	61		
2	E	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
2	F	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
2	G	1351	Total	C	N	O	S	0	0
			10705	6816	1854	1974	61		
2	H	1352	Total	C	N	O	S	0	0
			10710	6819	1855	1975	61		
2	I	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
2	J	1335	Total	C	N	O	S	0	0
			10581	6739	1837	1945	60		
2	K	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		
2	L	1353	Total	C	N	O	S	0	0
			10717	6823	1856	1977	61		
2	M	1353	Total	C	N	O	S	0	0
			10717	6823	1856	1977	61		
2	N	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
2	O	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		
2	P	1348	Total	C	N	O	S	0	0
			10681	6802	1851	1967	61		

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	V	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	W	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	X	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	Y	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	Z	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	a	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	b	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	c	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	d	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	e	63	Total 513	C 321	N 97	O 91	S 4	0	0
3	f	63	Total 513	C 321	N 97	O 91	S 4	0	0

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	260	Total 2091	C 1344	N 365	O 371	S 11	0	0
4	j	290	Total 2325	C 1485	N 411	O 417	S 12	0	0
4	m	290	Total 2325	C 1485	N 411	O 417	S 12	0	0
4	p	290	Total 2325	C 1485	N 411	O 417	S 12	0	0
4	s	290	Total 2325	C 1485	N 411	O 417	S 12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	292	Total	C	N	O	S	0	0
			2316	1490	399	409	18		
5	i	285	Total	C	N	O	S	0	0
			2258	1454	386	401	17		
5	k	292	Total	C	N	O	S	0	0
			2317	1491	399	408	19		
5	l	303	Total	C	N	O	S	0	0
			2406	1541	419	428	18		
5	n	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
5	o	291	Total	C	N	O	S	0	0
			2311	1484	398	411	18		
5	q	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
5	r	304	Total	C	N	O	S	0	0
			2411	1544	420	429	18		
5	t	296	Total	C	N	O	S	0	0
			2342	1505	403	415	19		
5	u	304	Total	C	N	O	S	0	0
			2411	1544	420	429	18		

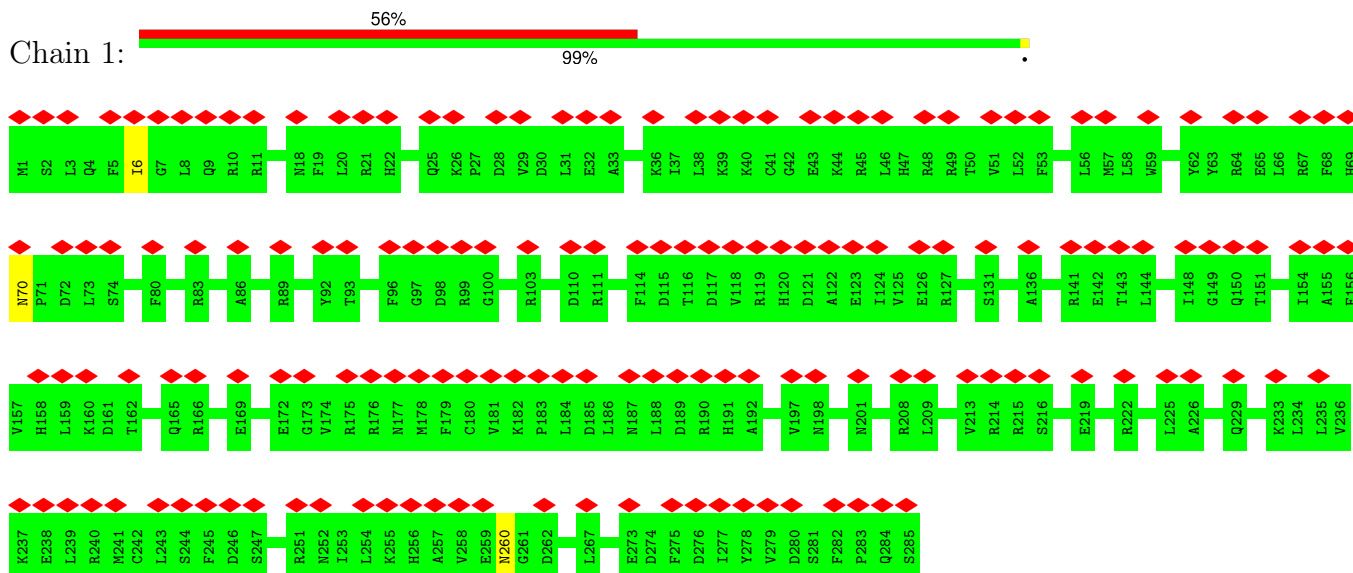
3 Residue-property plots

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.

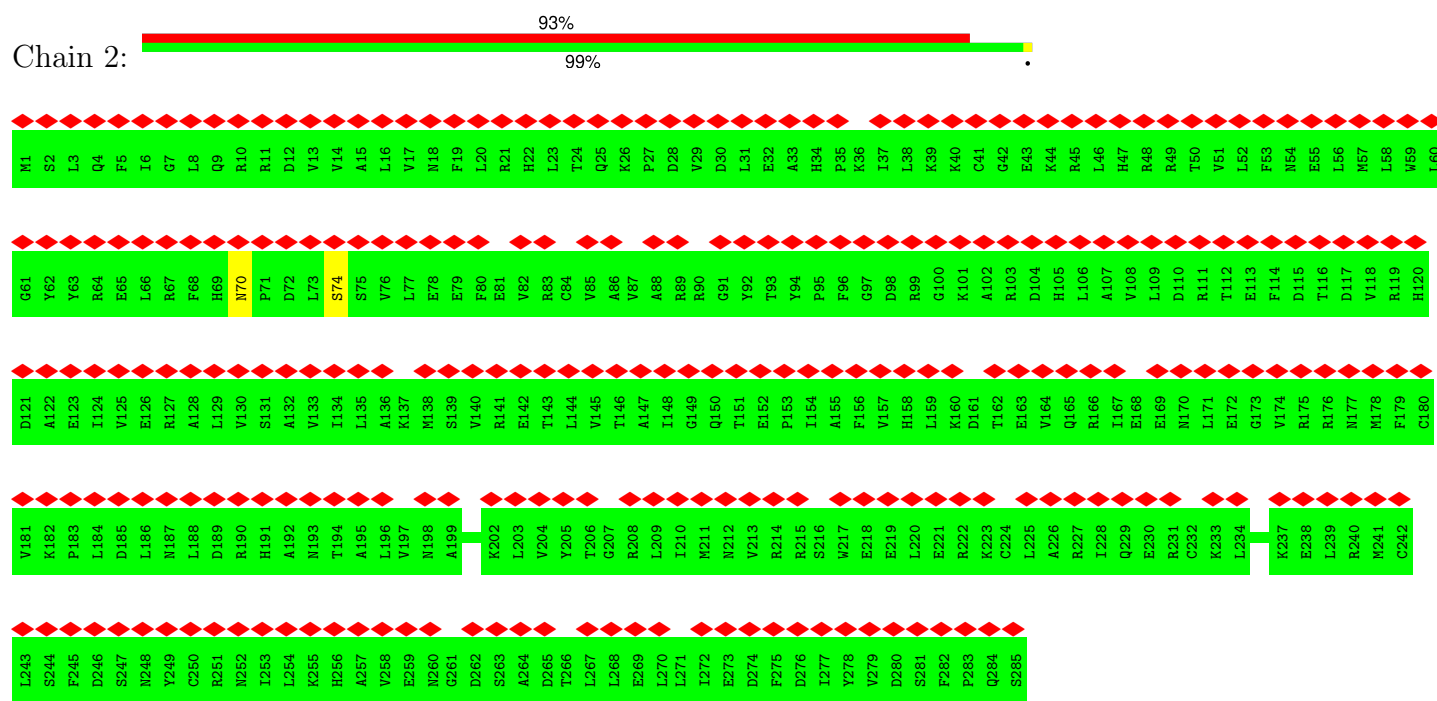
- Molecule 1: Tegument protein pp150



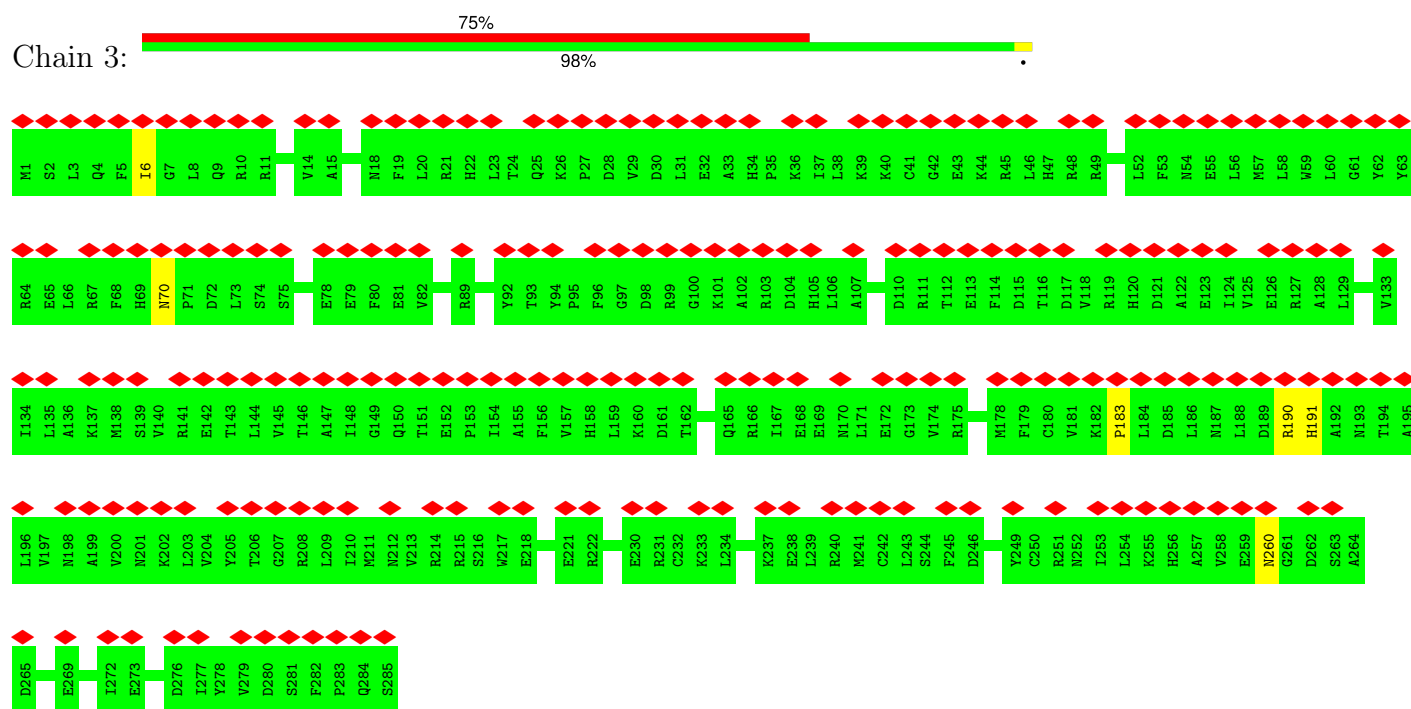
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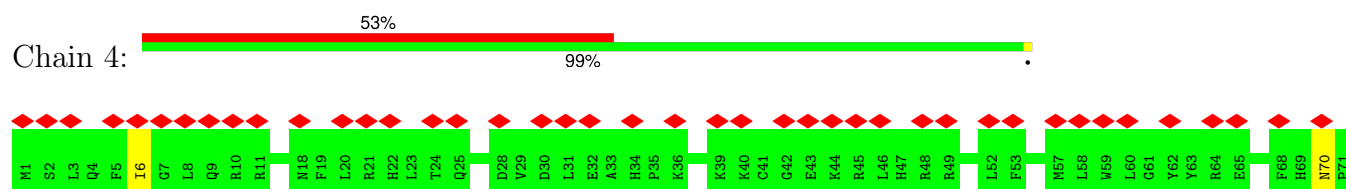
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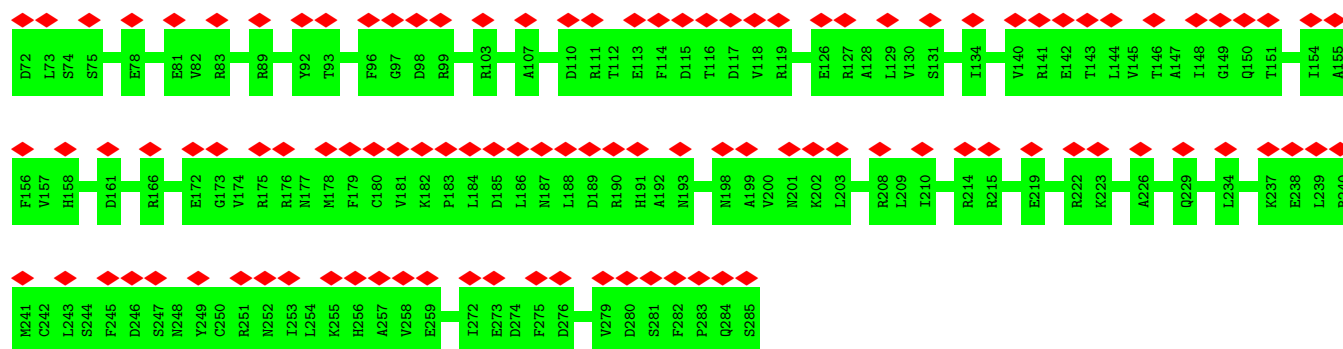


• Molecule 1: Tegument protein pp150



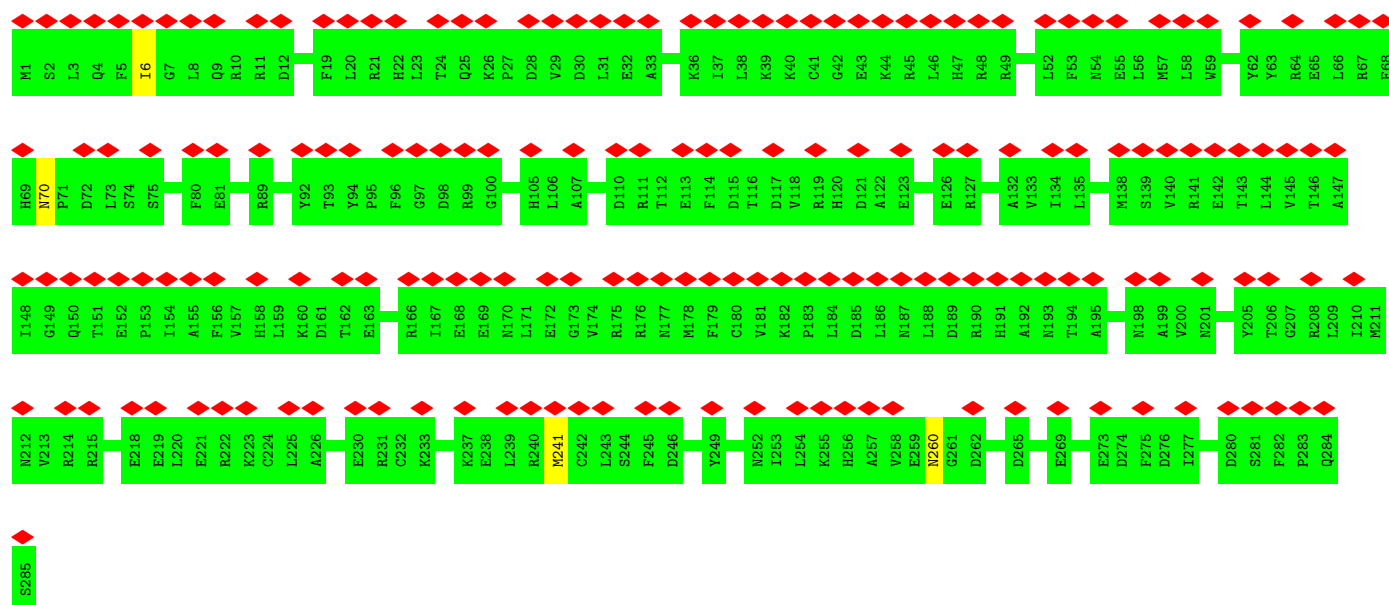
• Molecule 1: Tegument protein pp150





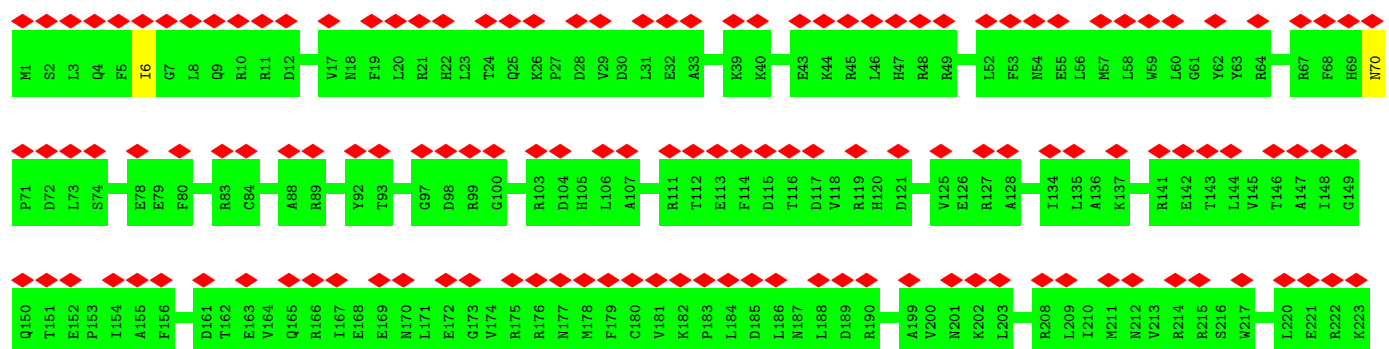
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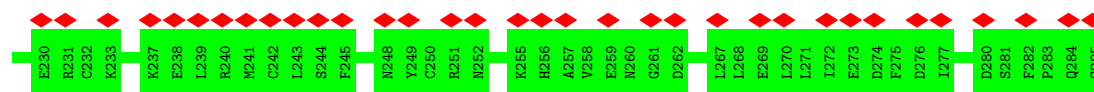
Chain 5: 63% 99%



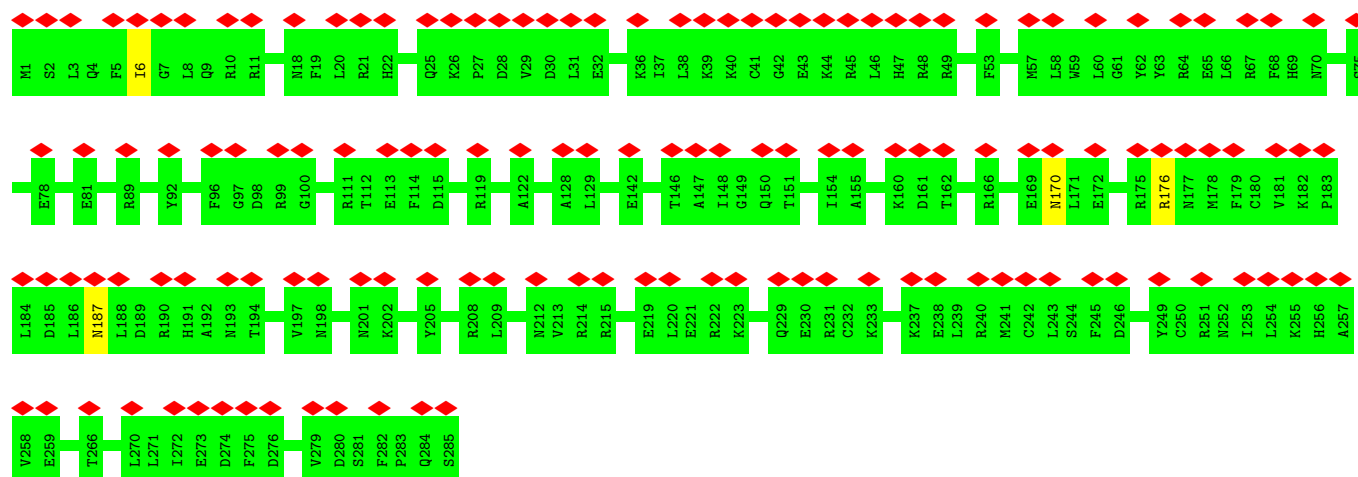
- Molecule 1: Tegument protein pp150

Chain 6: 60% 99%

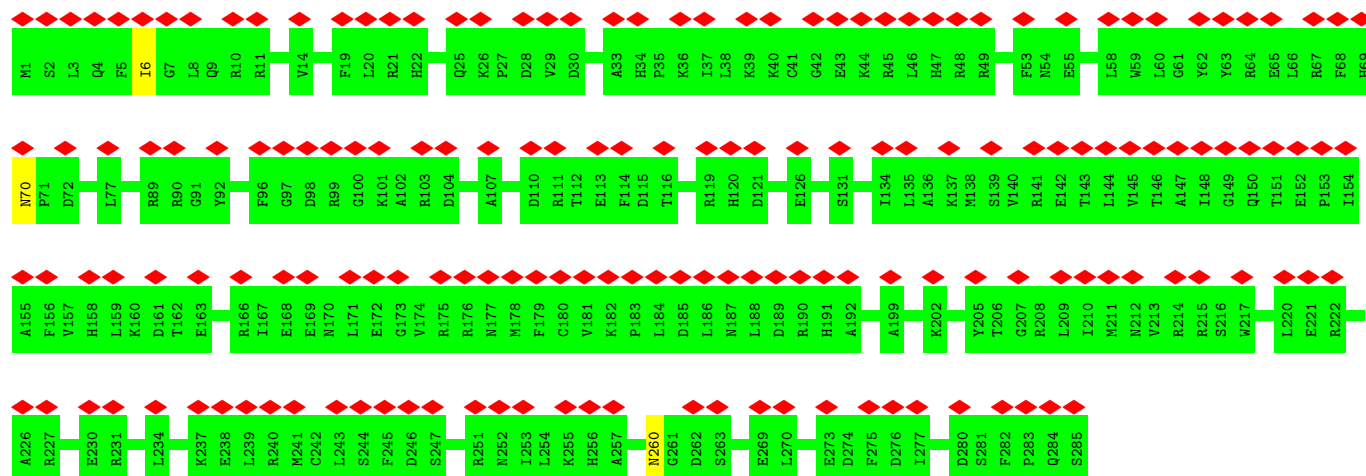




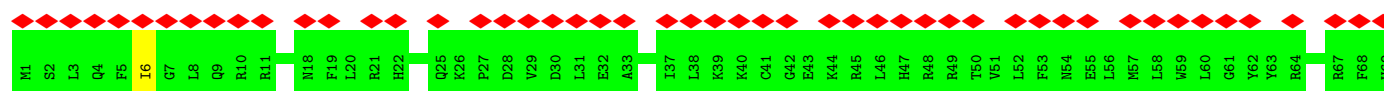
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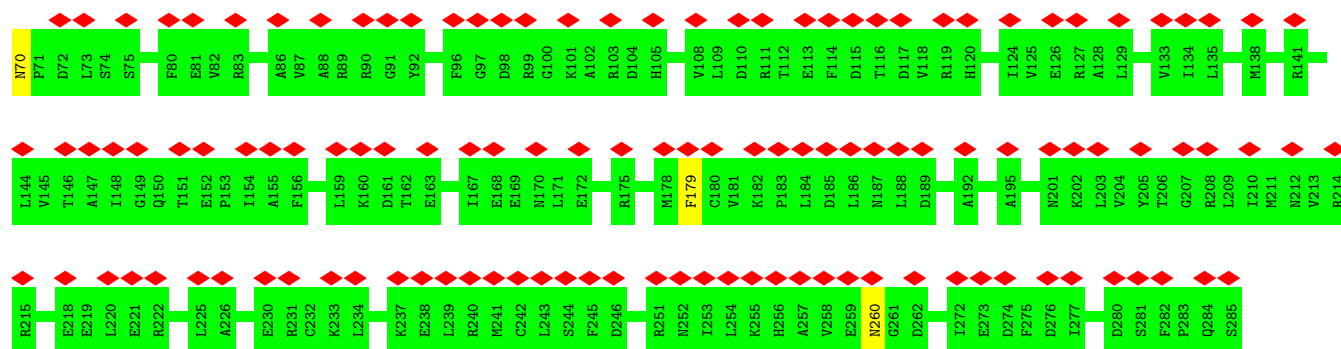


- Molecule 1: Tegument protein pp150

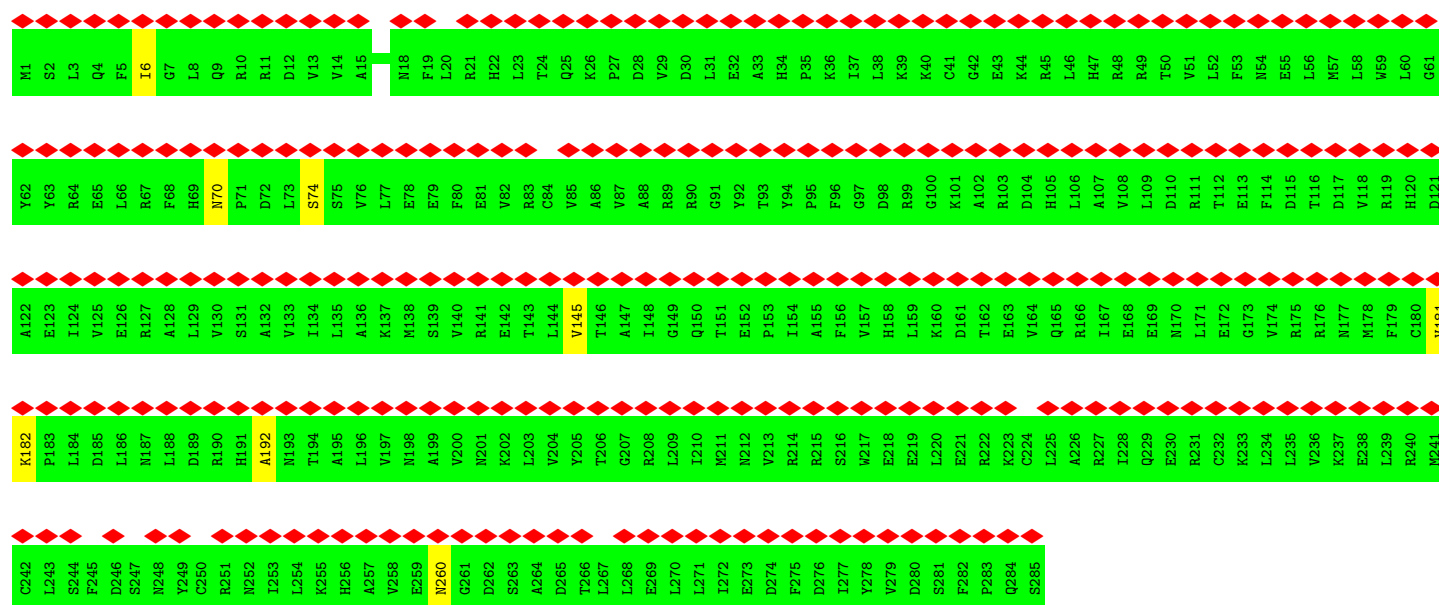


- Molecule 1: Tegument protein pp150

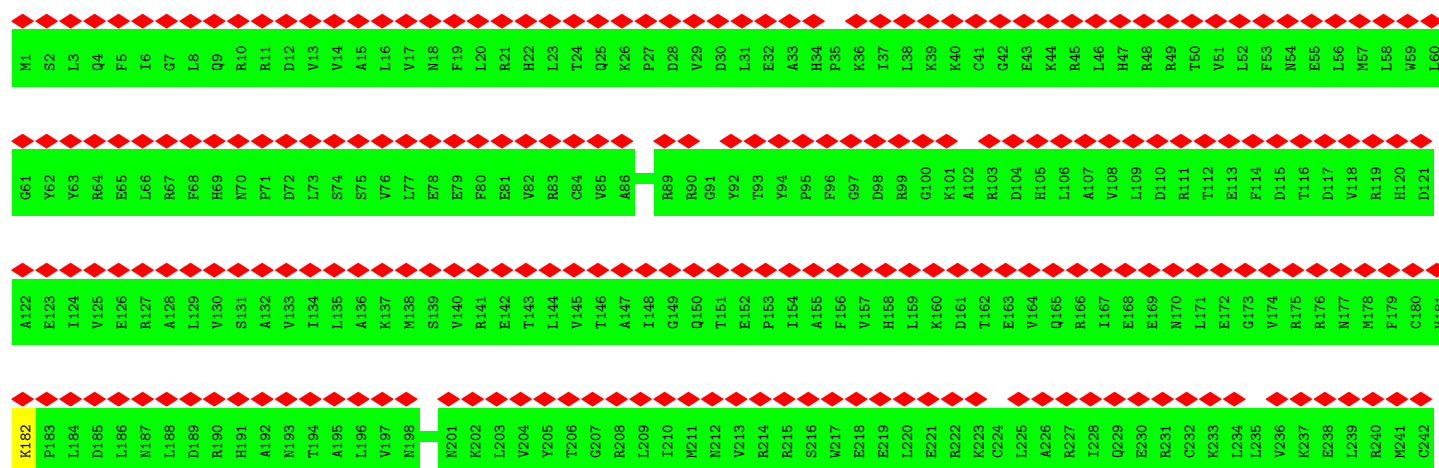


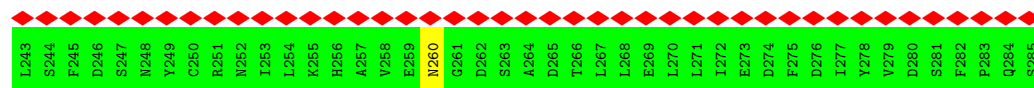


• Molecule 1: Tegument protein pp150

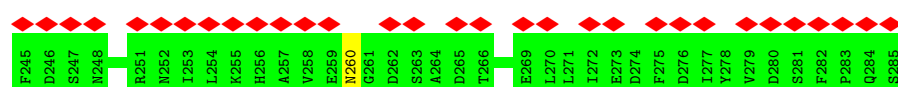
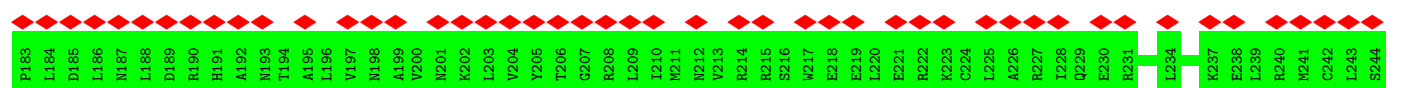
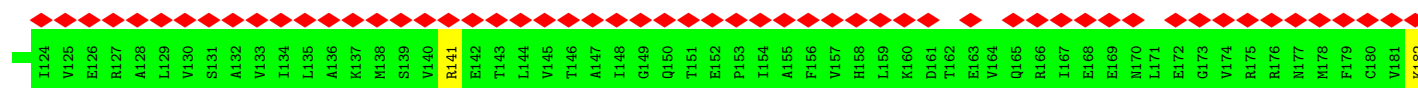
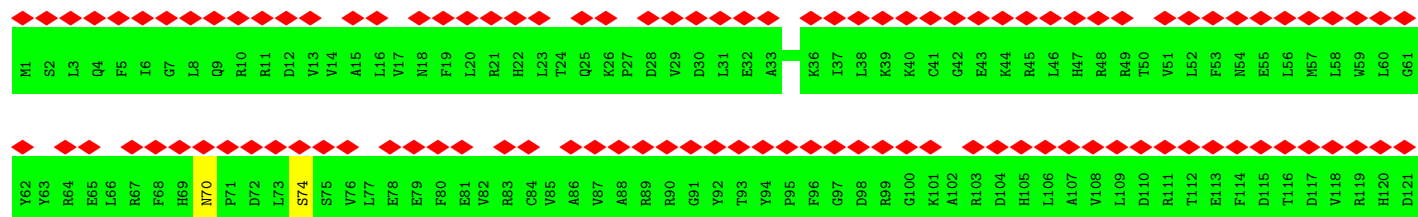
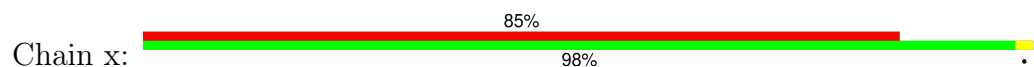


• Molecule 1: Tegument protein pp150

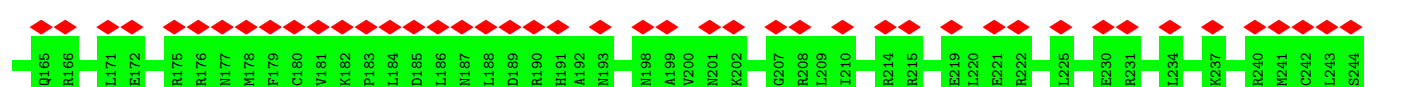
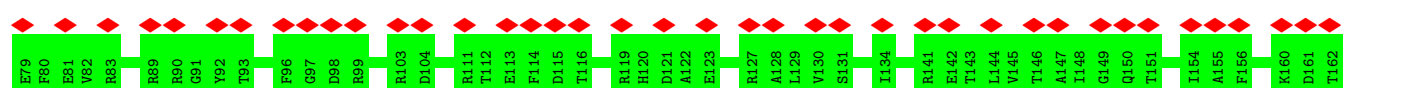
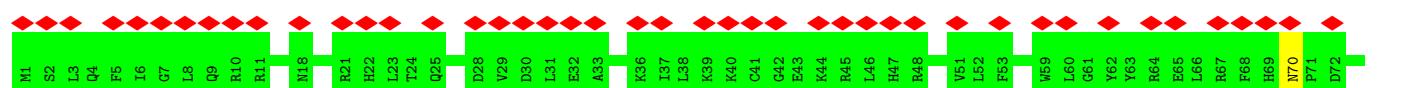




• Molecule 1: Tegument protein pp150

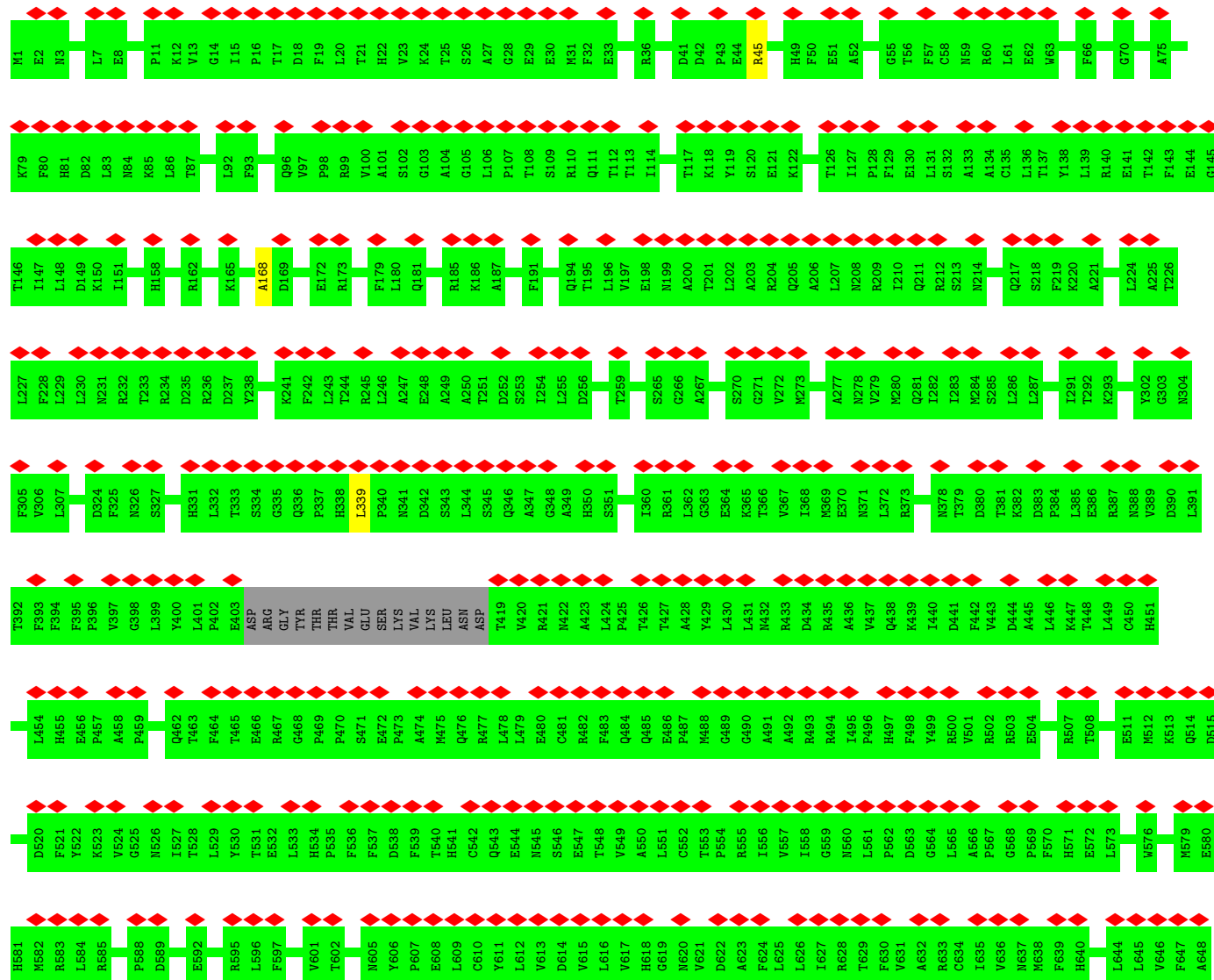


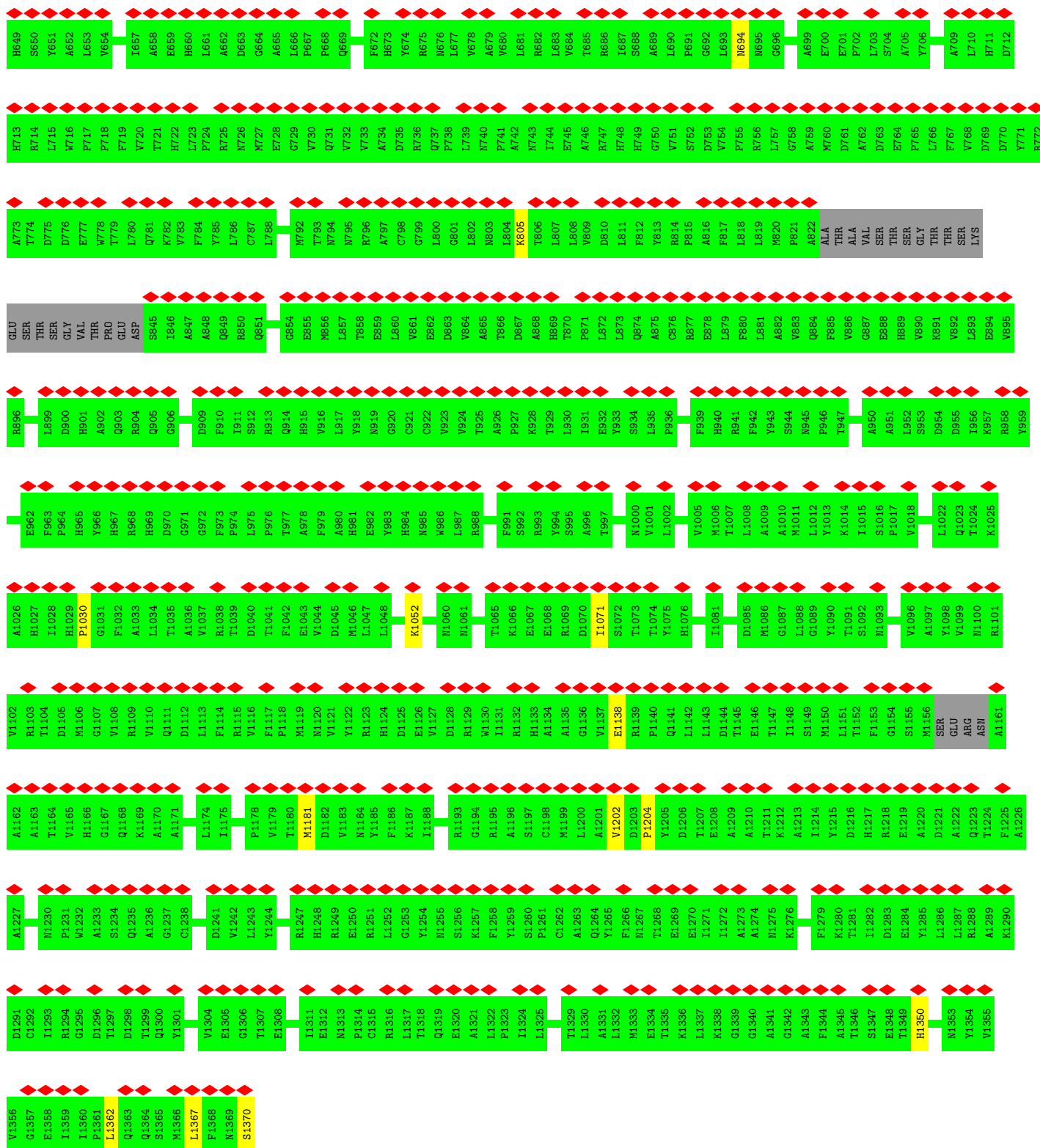
• Molecule 1: Tegument protein pp150



• Molecule 1: Tegument protein pp150



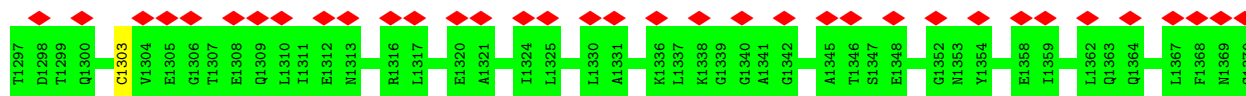
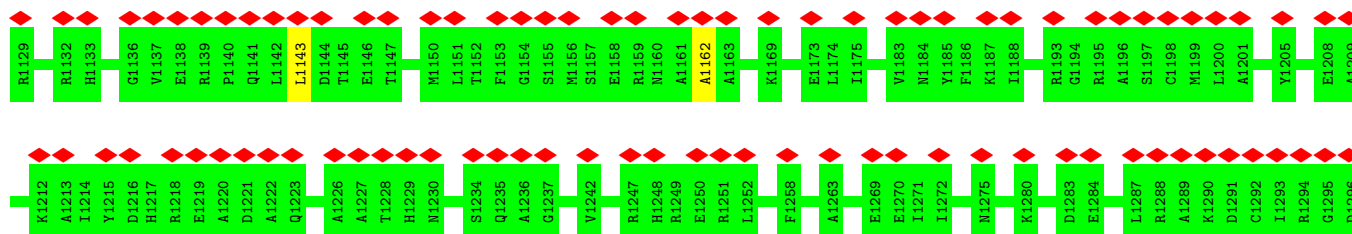




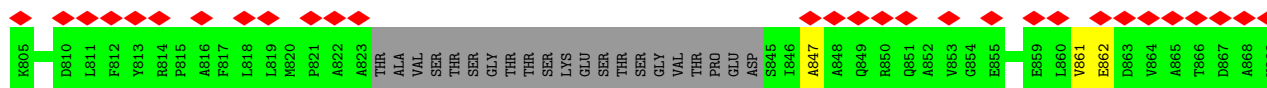
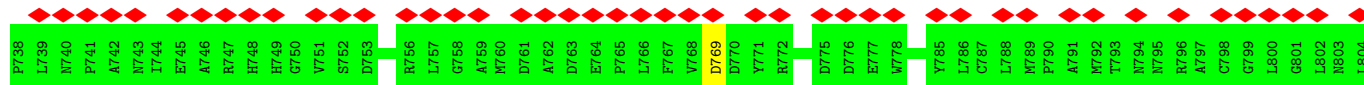
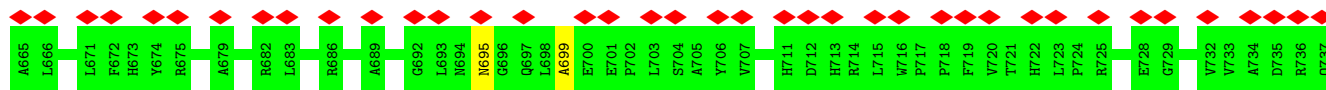
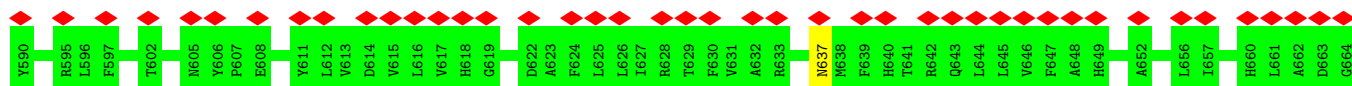
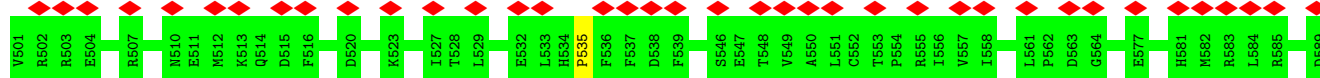
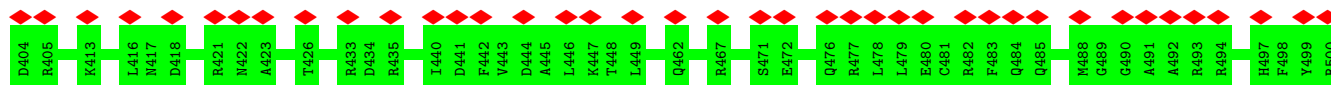
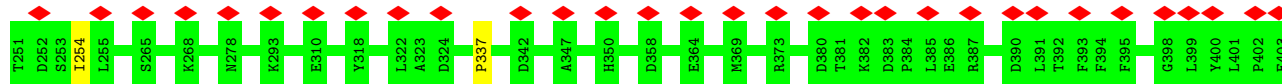
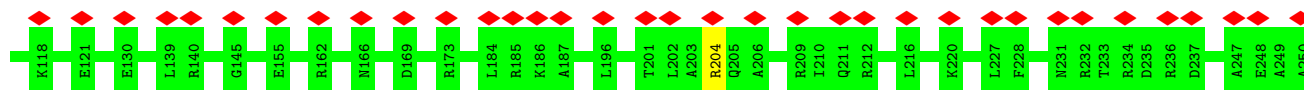
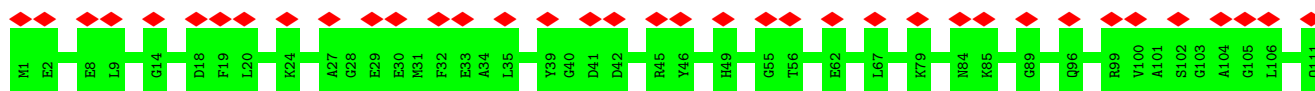
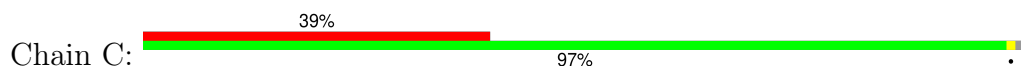
• Molecule 2: Major capsid protein

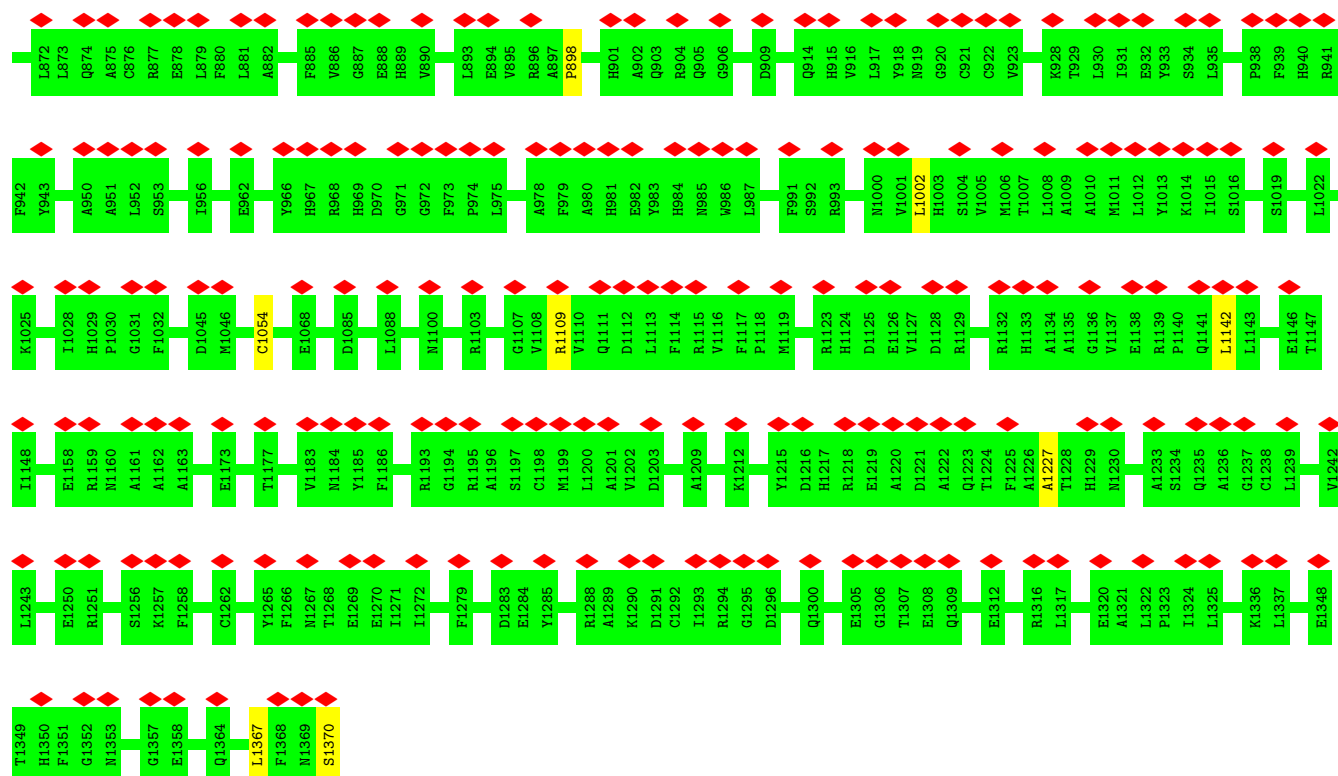


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S345	Q346	A347	G348	A349	H350	S351	L352	D358	V359	I360	R361	E364	N371	L372	R373	N378	T379	D380	T381	K382	D383	P384	L385	D390	L391	T392	F393	F394	F395	G398	L399	E403	D404	R405	E411	S412	K413	V414	K415	L416	N417	D418	R421	N422	A423	N510	L424	P425	T426	R433						
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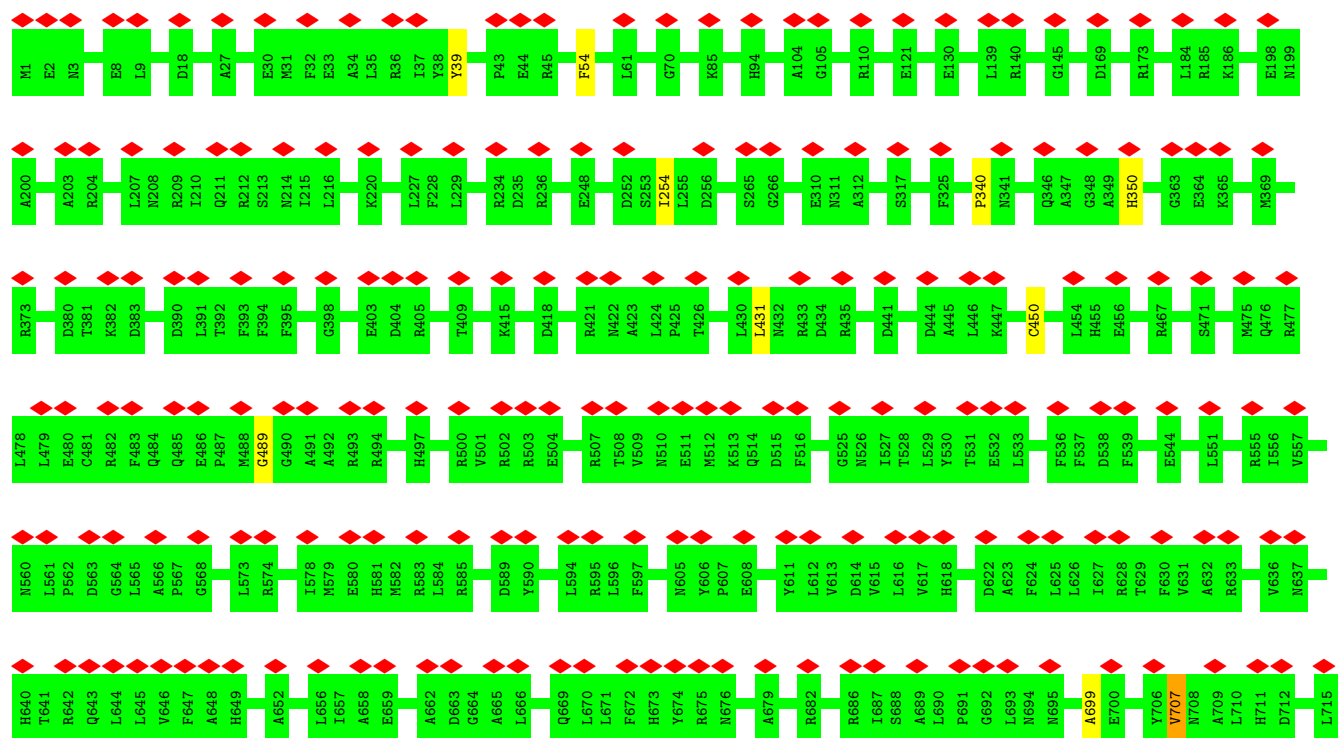


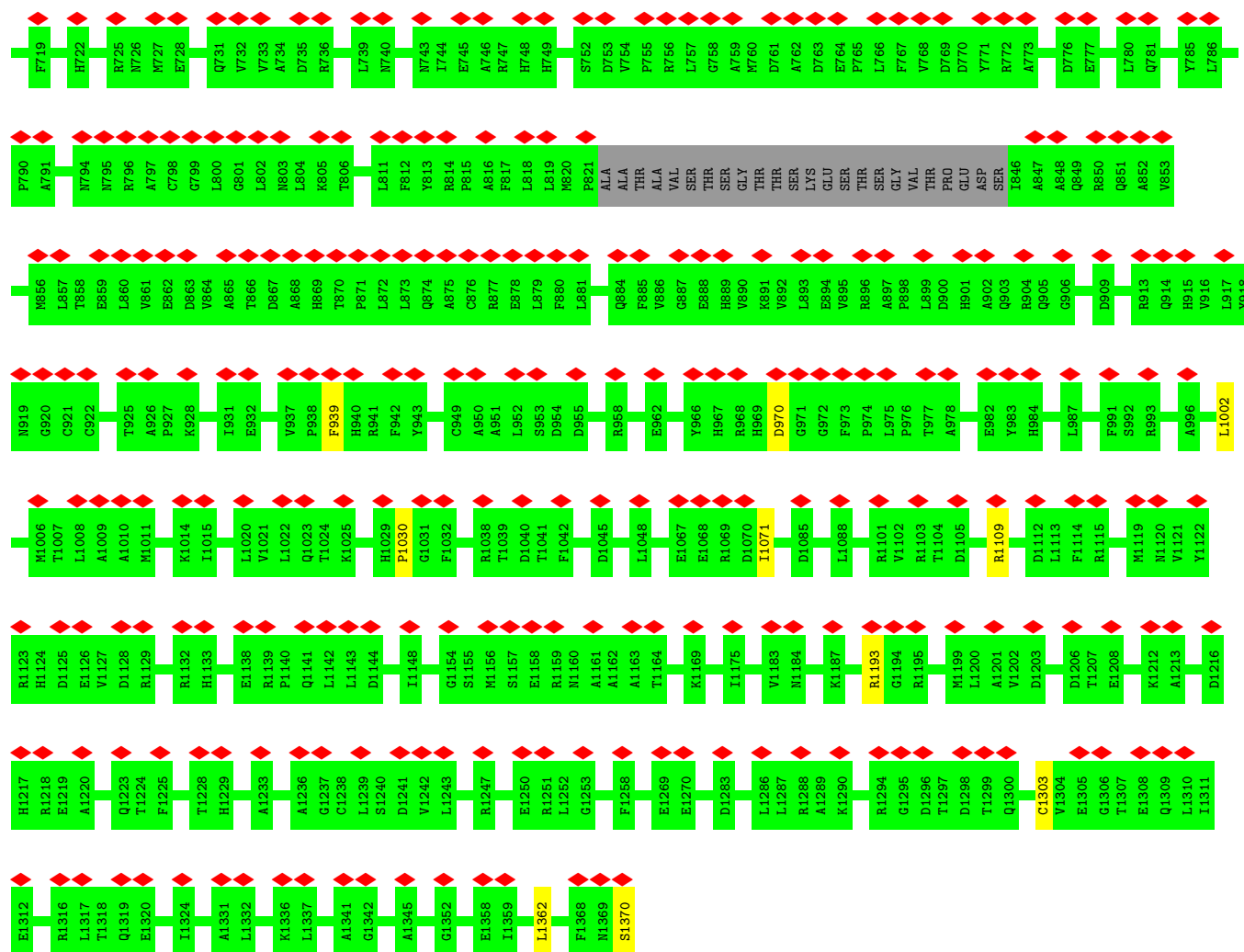
• Molecule 2: Major capsid protein



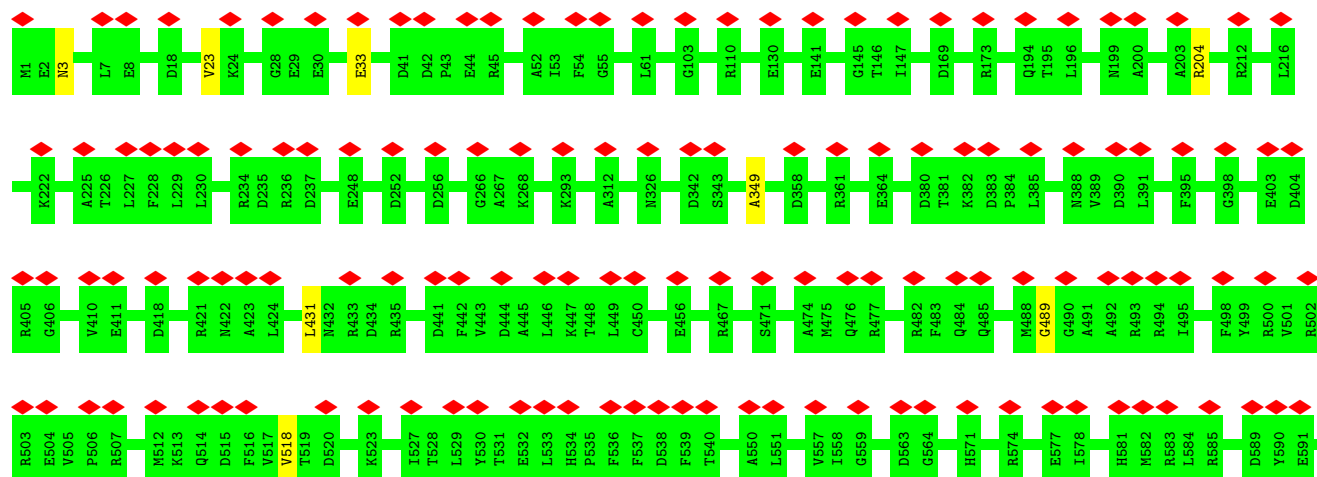


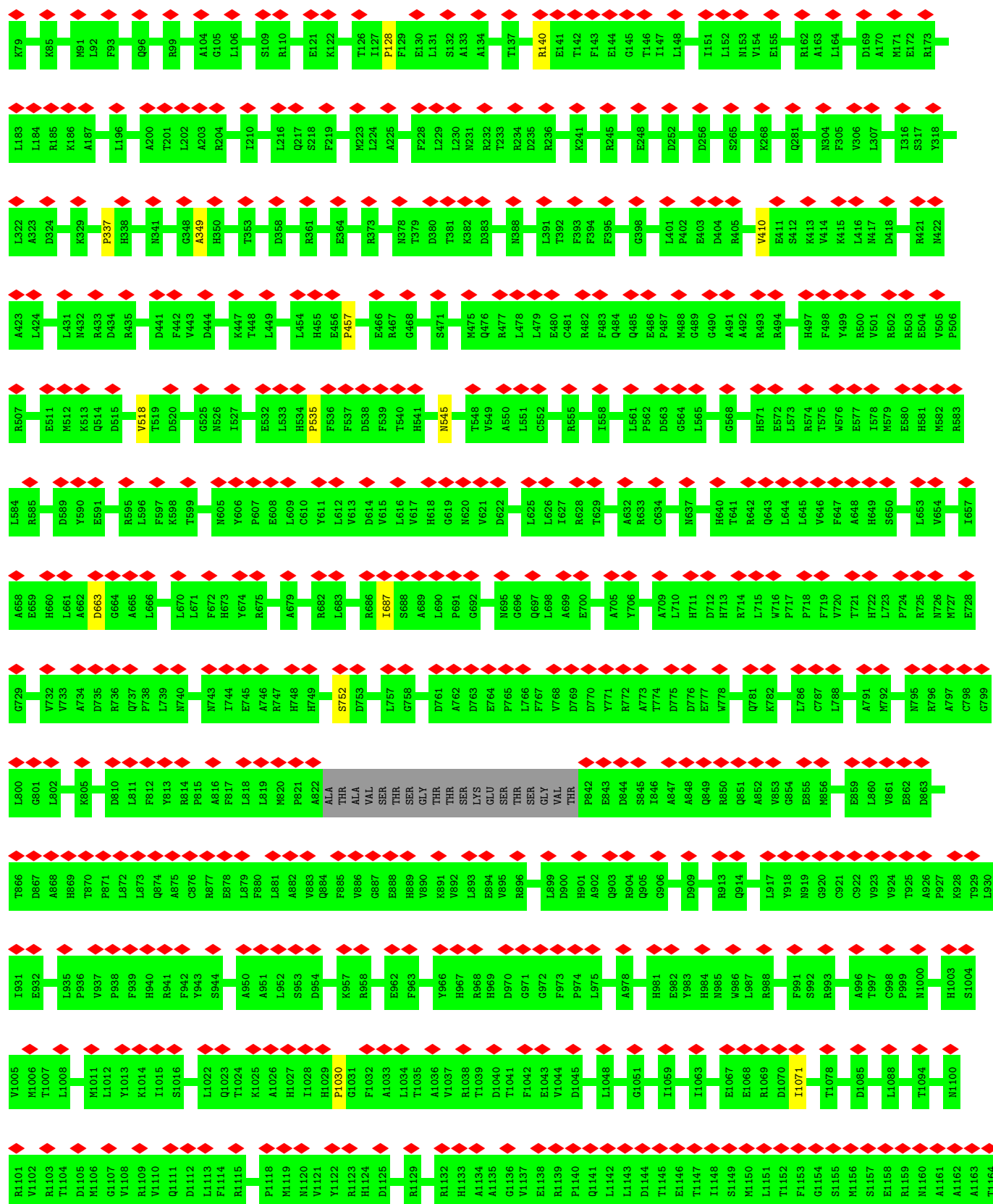
• Molecule 2: Major capsid protein

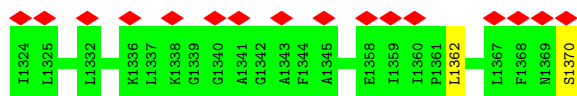
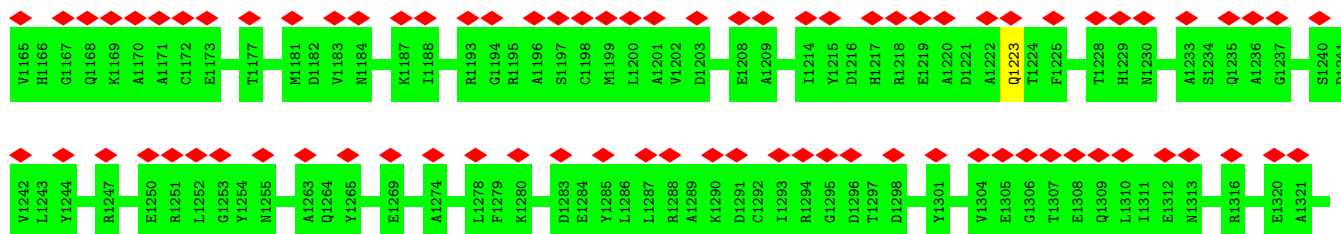




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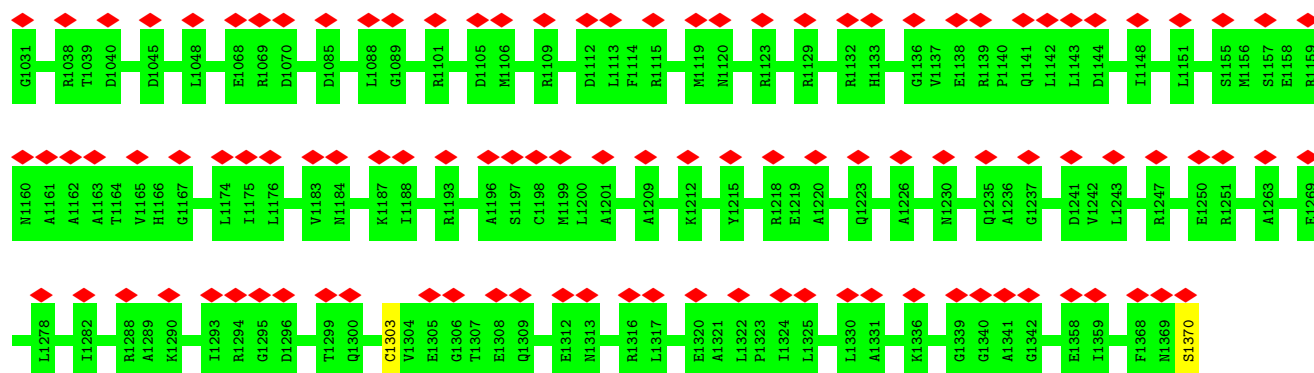






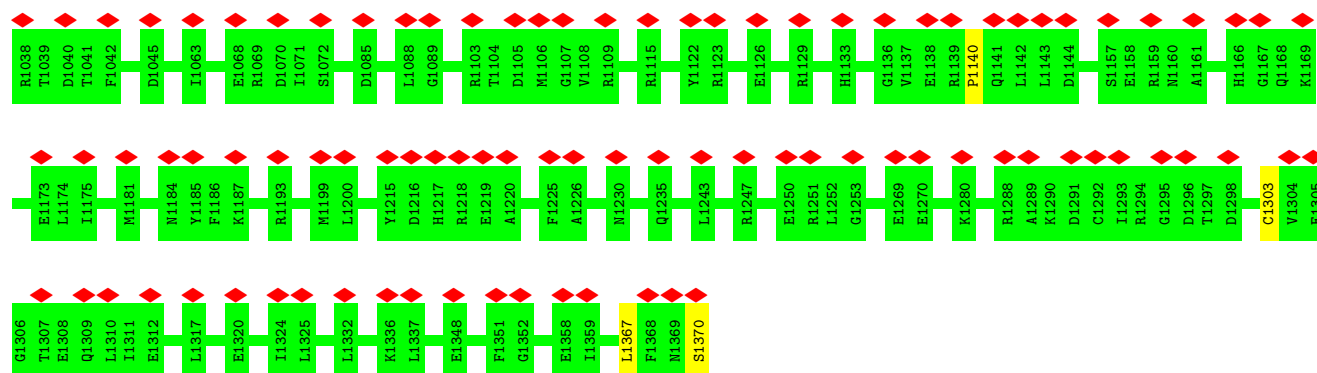
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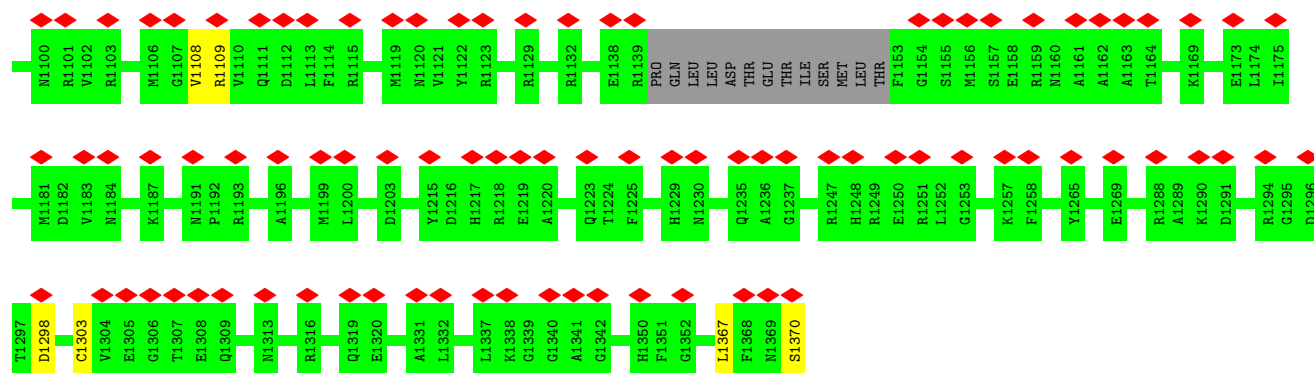
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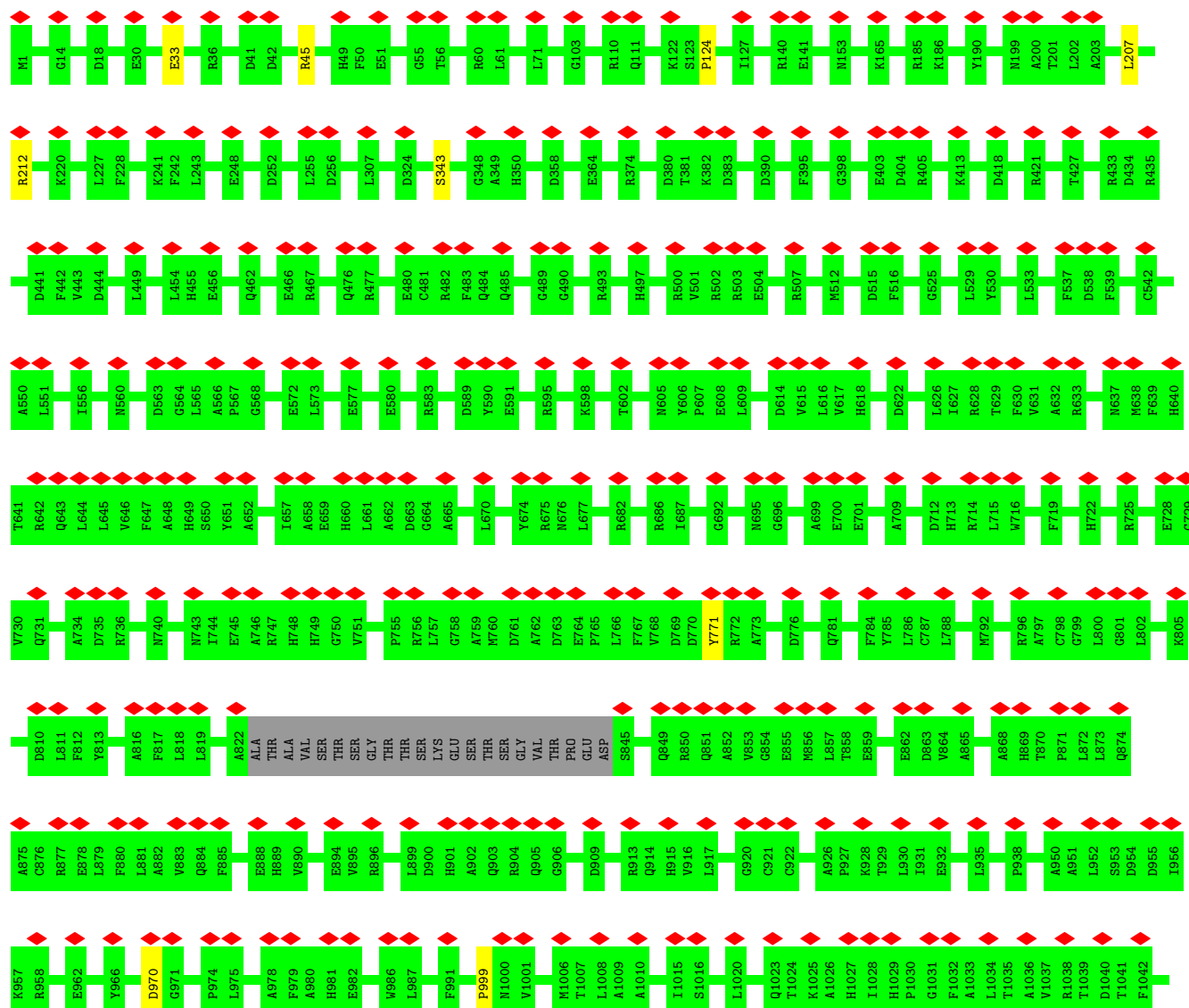


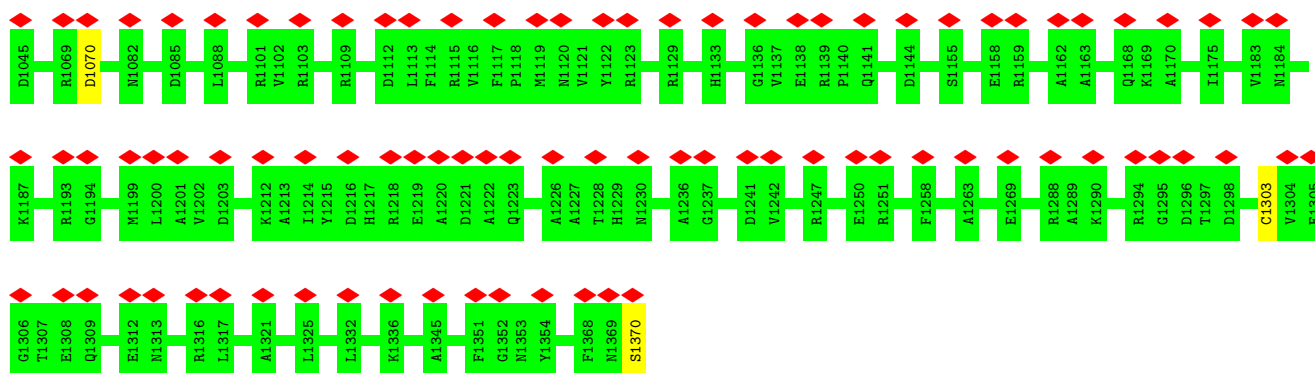
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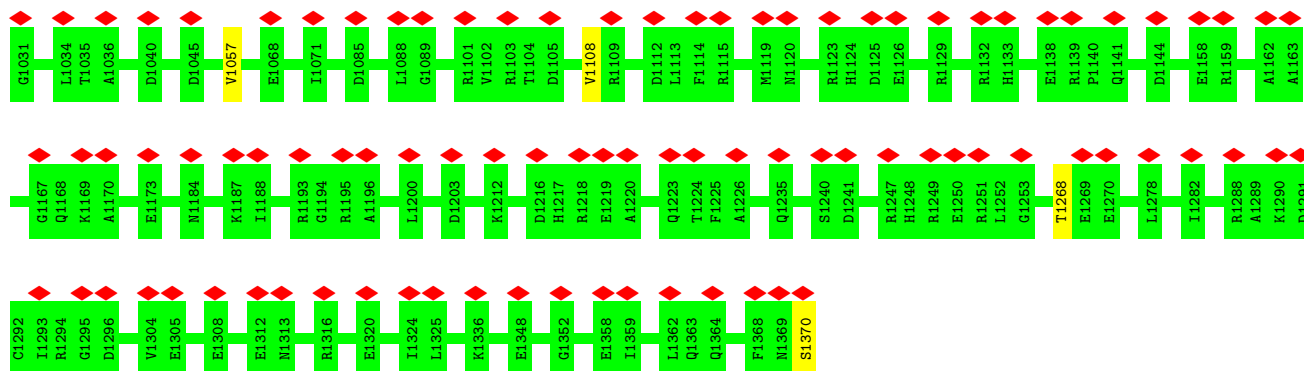
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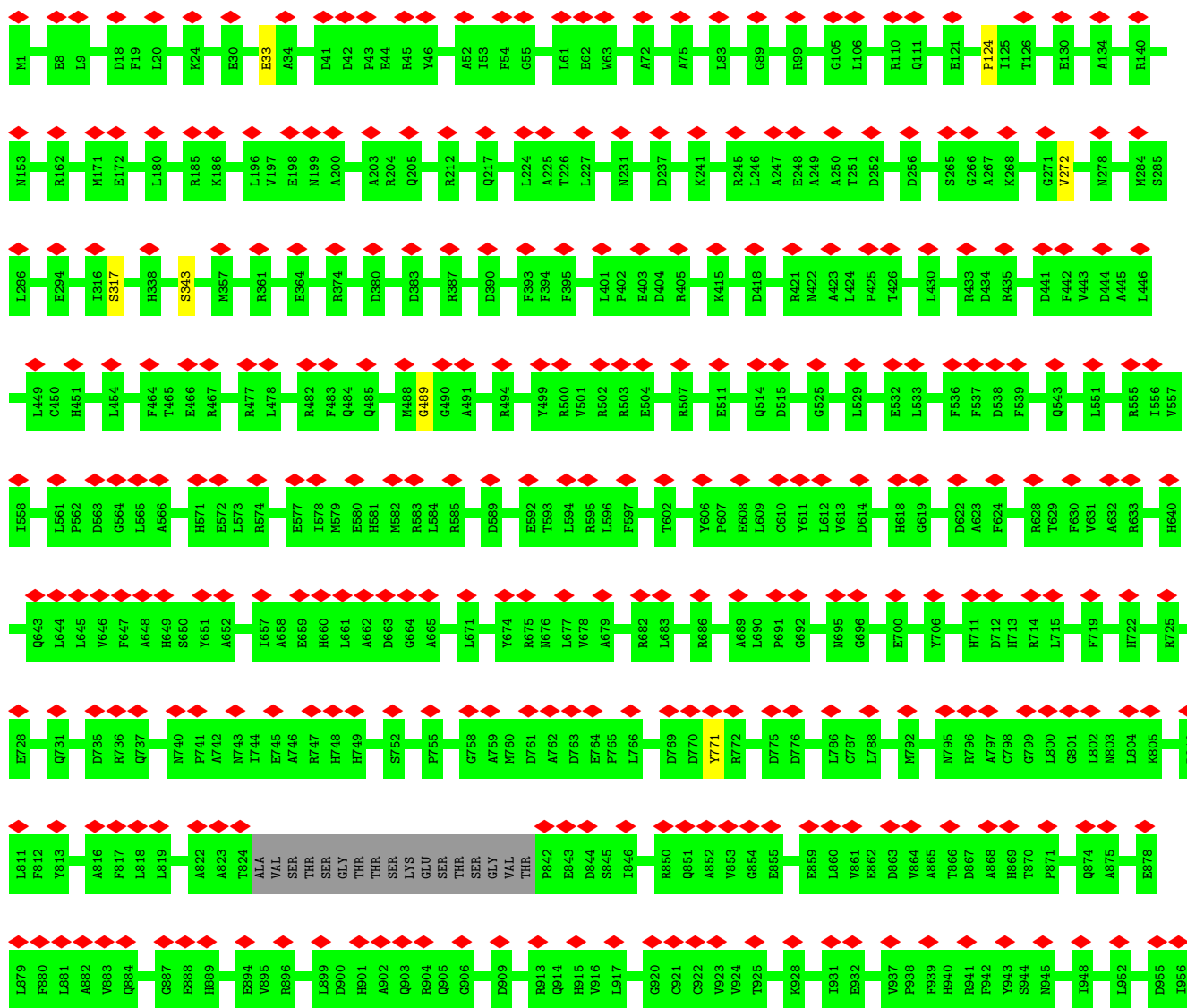


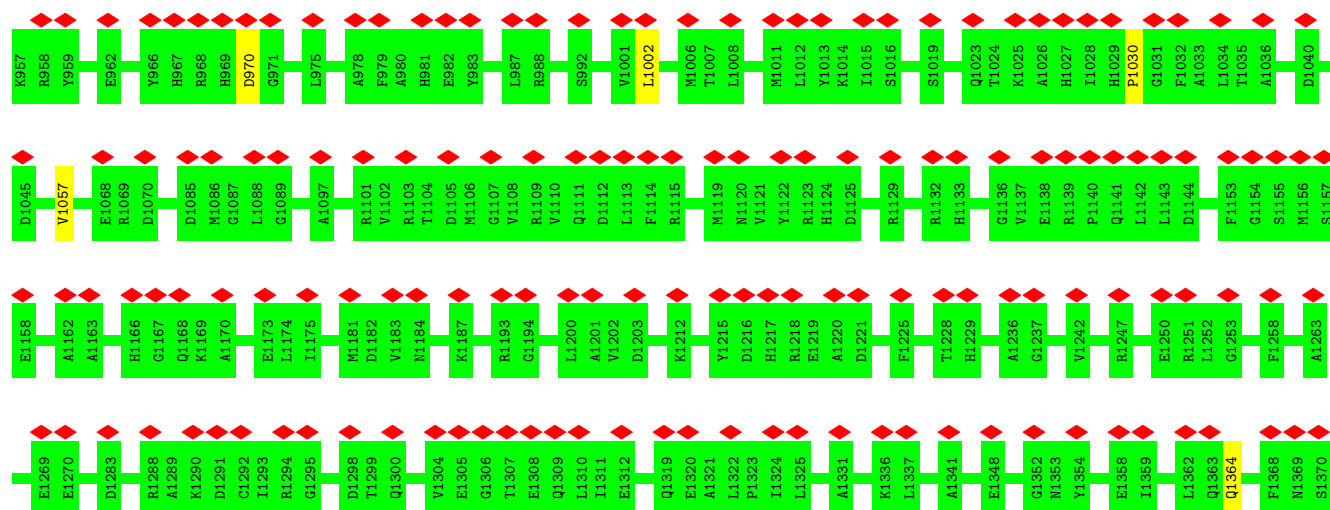
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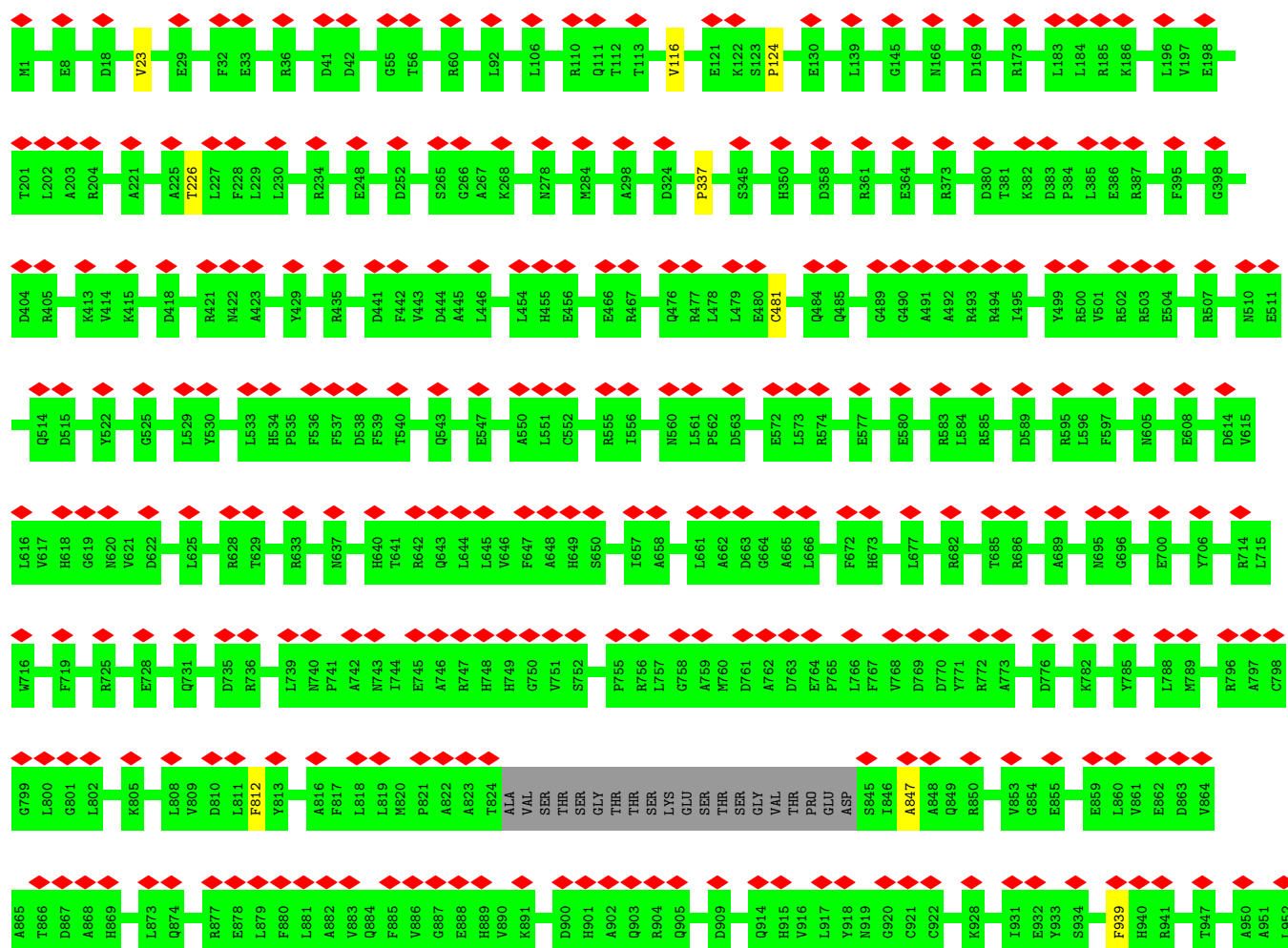


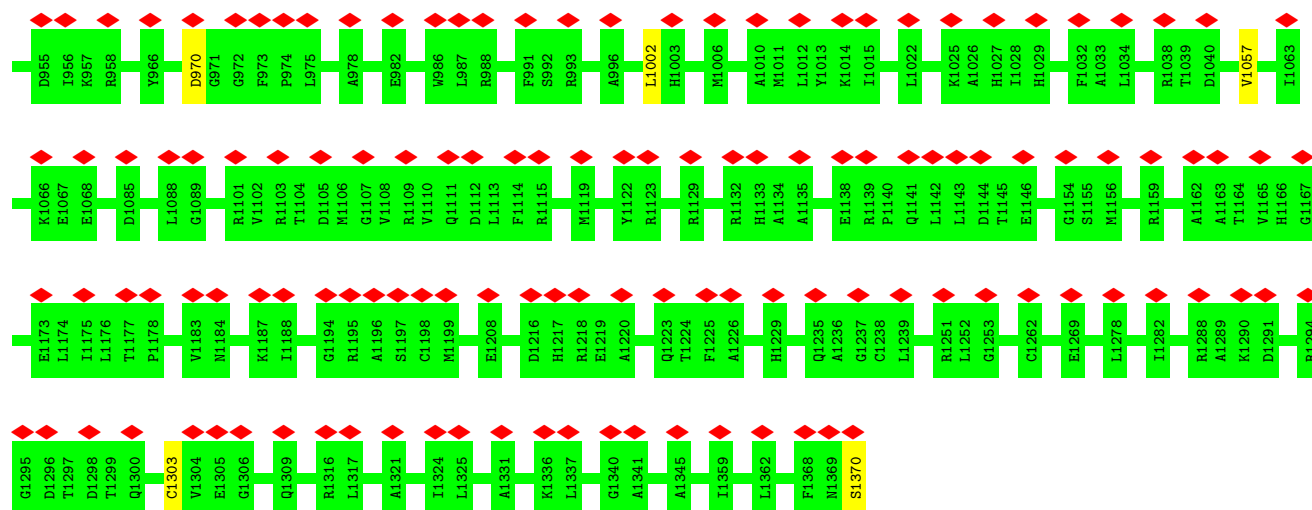
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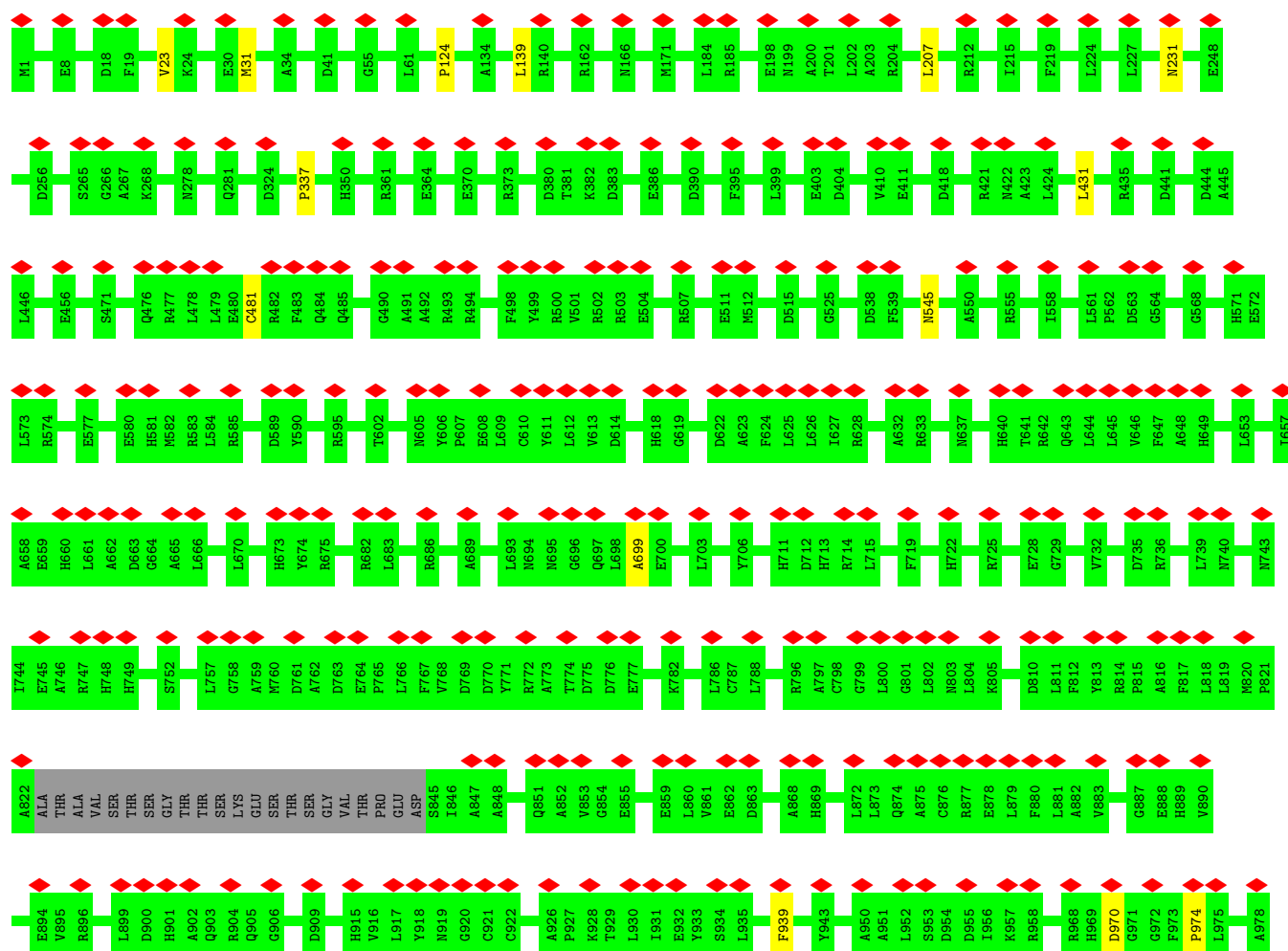


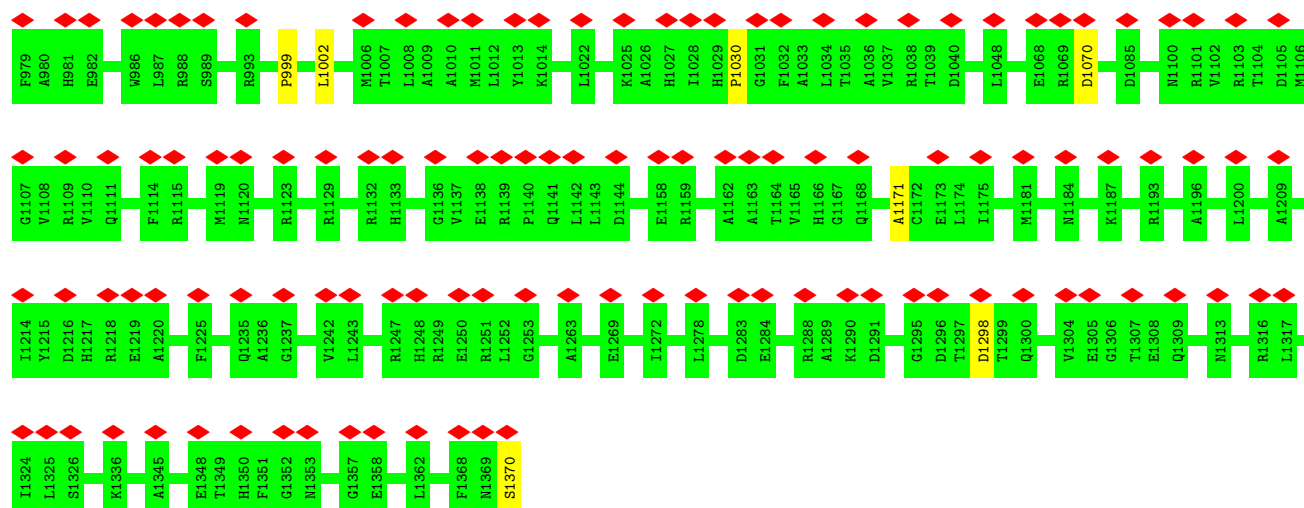
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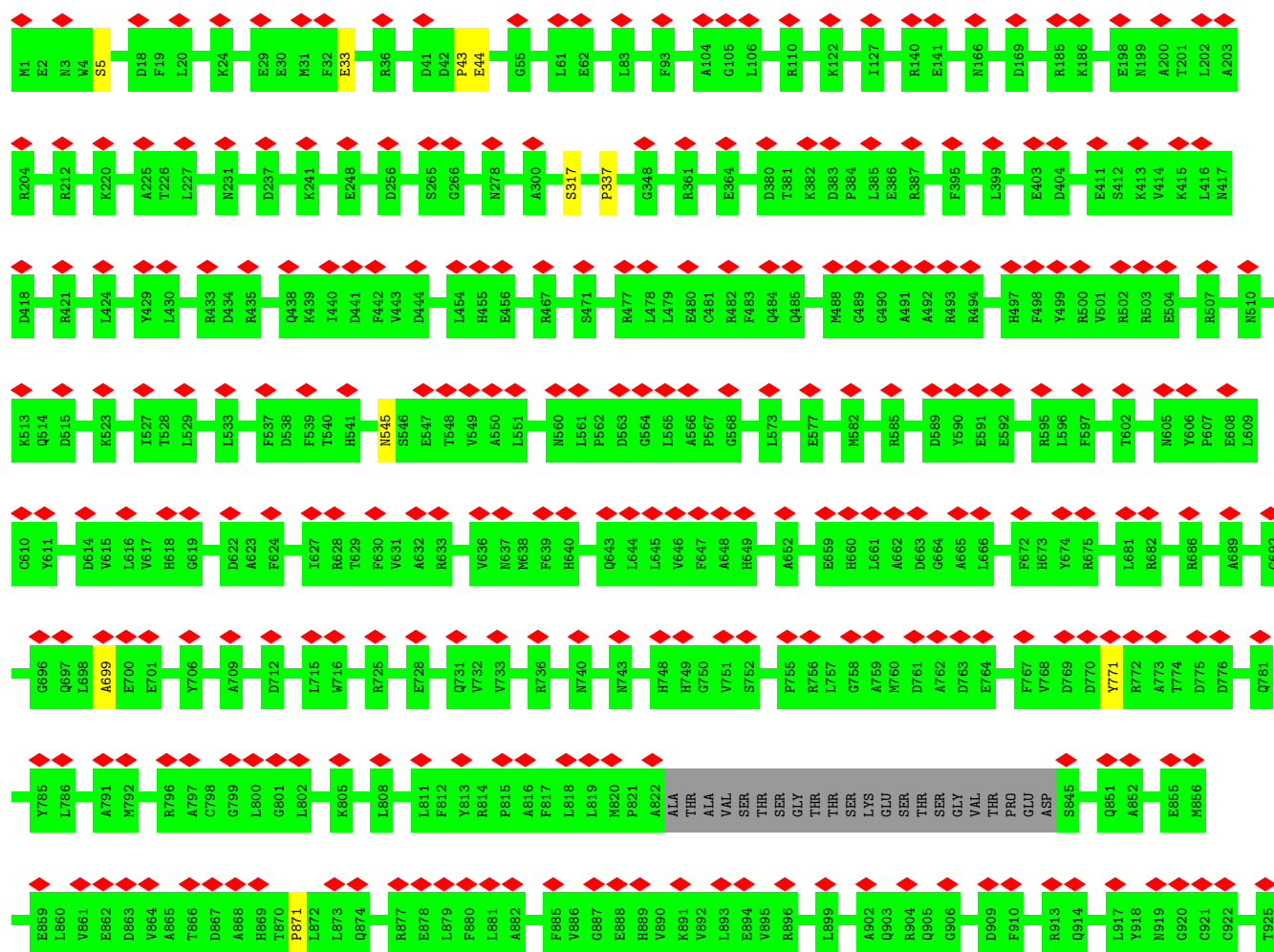


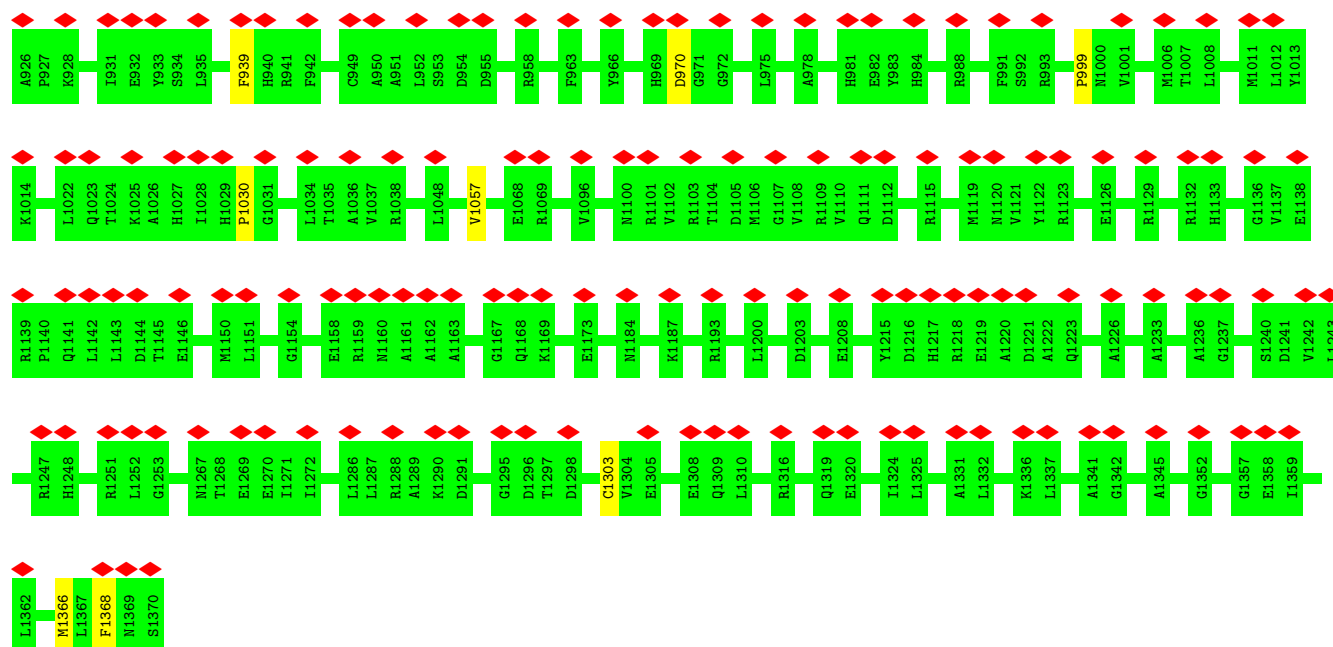
• Molecule 2: Major capsid protein



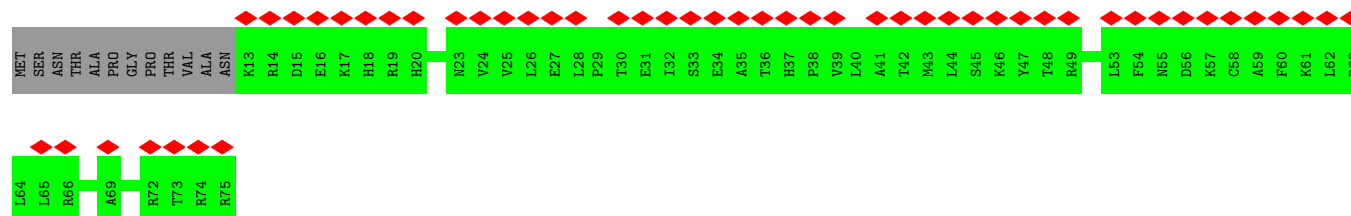
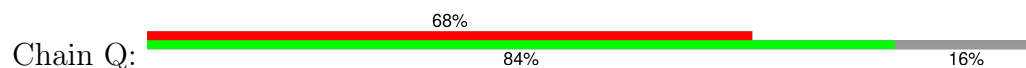


• Molecule 2: Major capsid protein

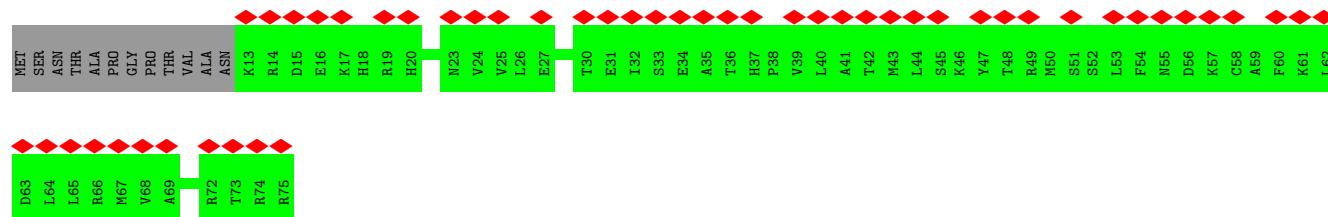
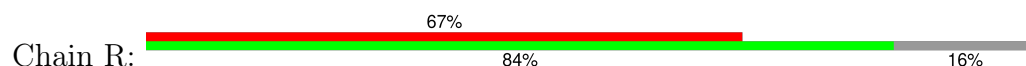




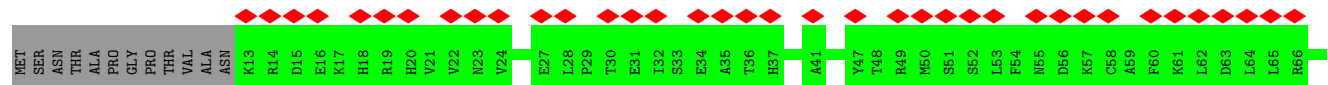
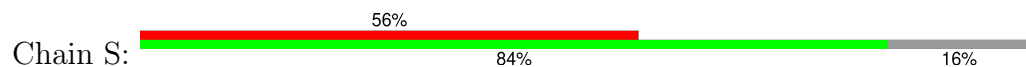
• Molecule 3: Small capsomere-interacting protein



• Molecule 3: Small capsomere-interacting protein

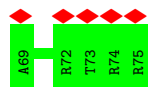
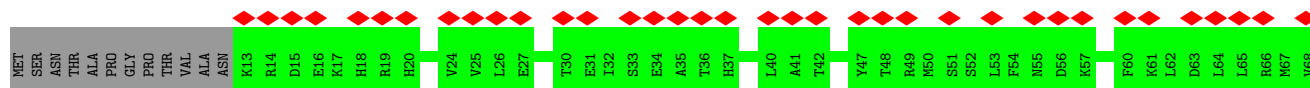
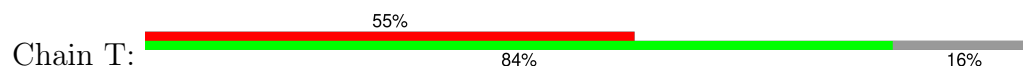


• Molecule 3: Small capsomere-interacting protein

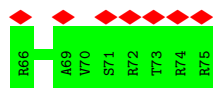
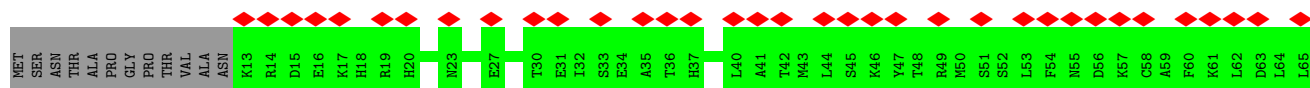
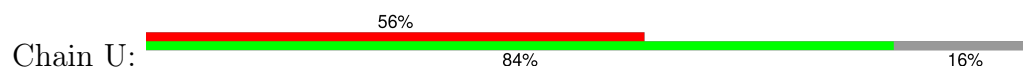




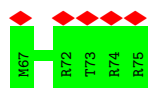
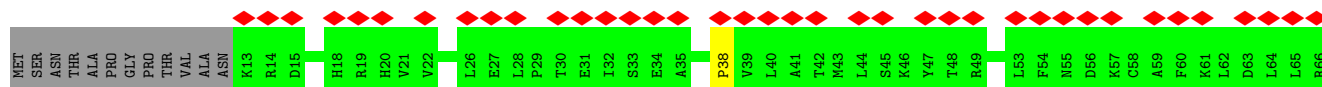
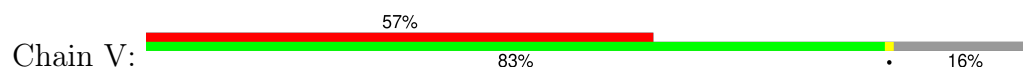
- Molecule 3: Small capsomere-interacting protein



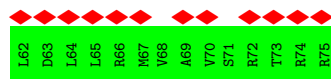
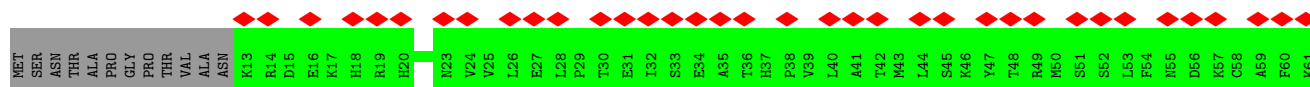
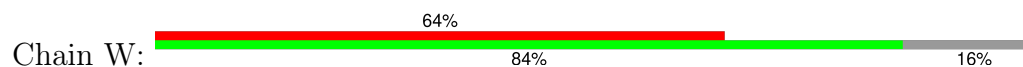
- Molecule 3: Small capsomere-interacting protein



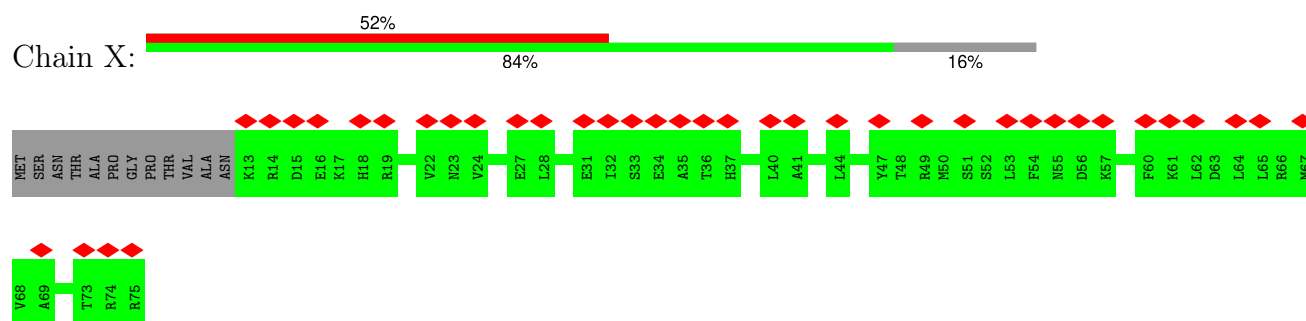
- Molecule 3: Small capsomere-interacting protein



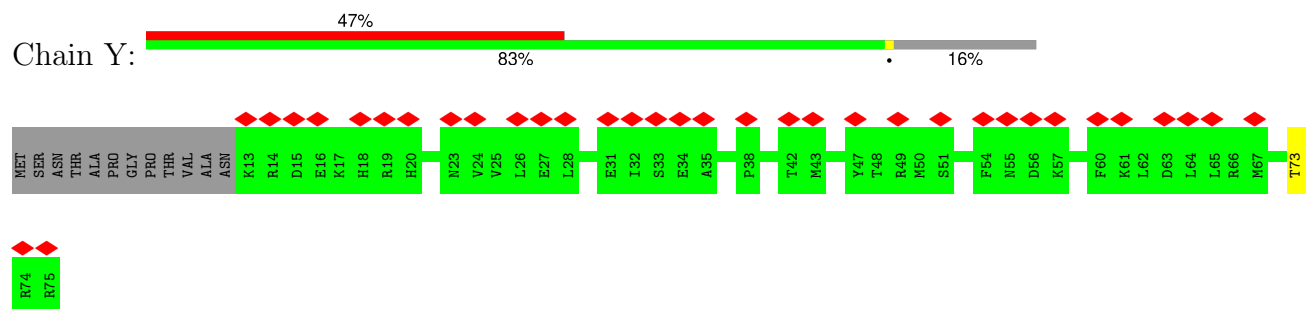
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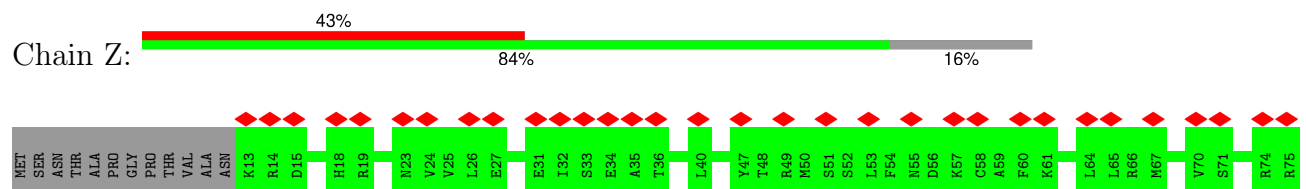
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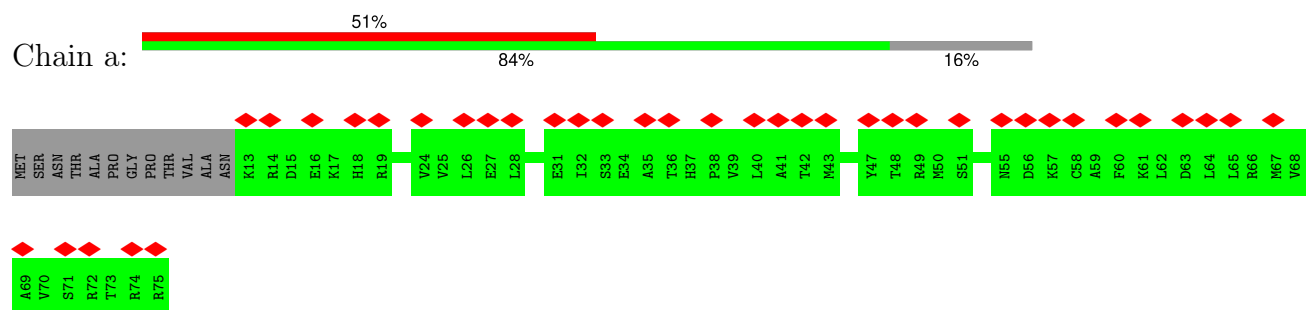
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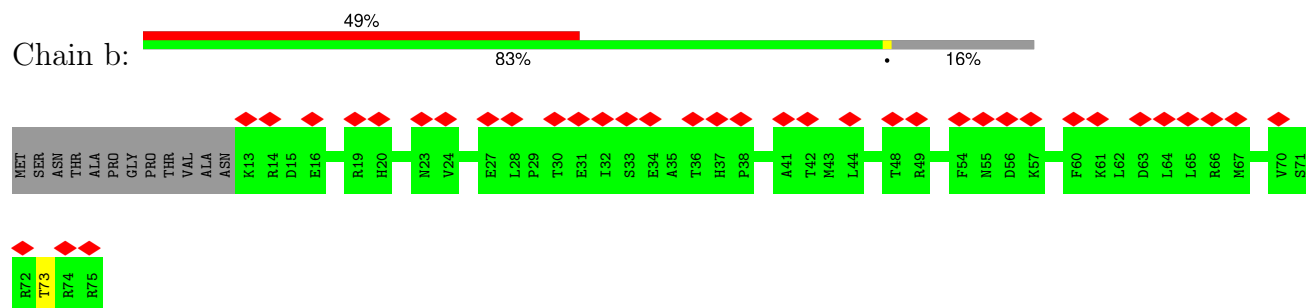
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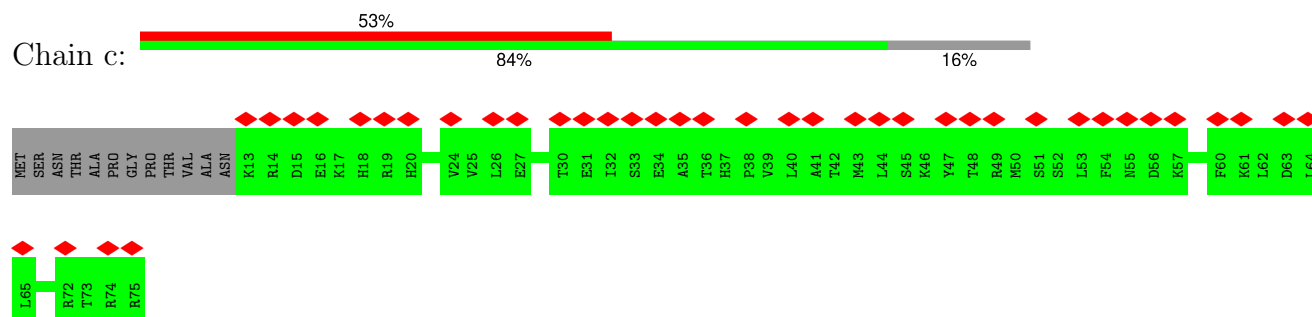
- Molecule 3: Small capsomere-interacting protein



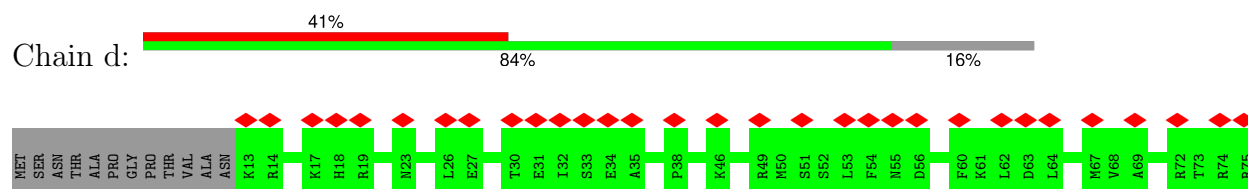
- Molecule 3: Small capsomere-interacting protein



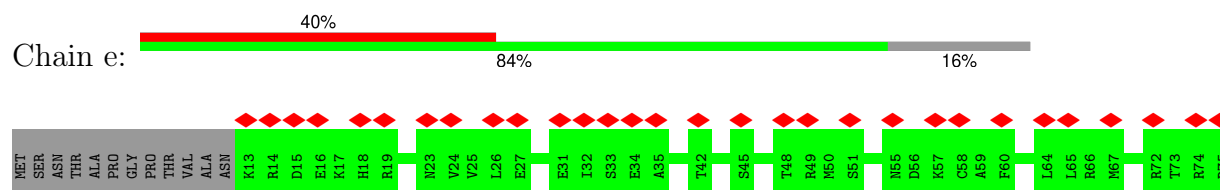
- Molecule 3: Small capsomere-interacting protein



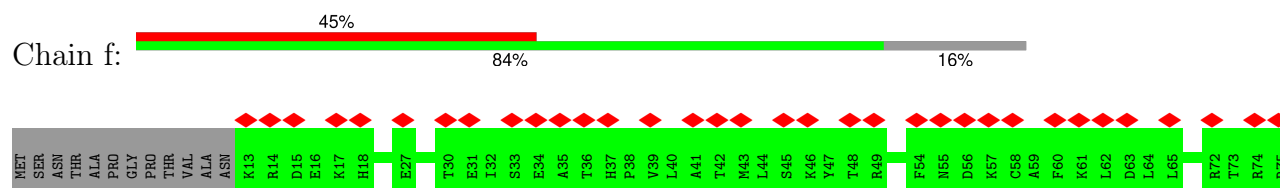
- Molecule 3: Small capsomere-interacting protein



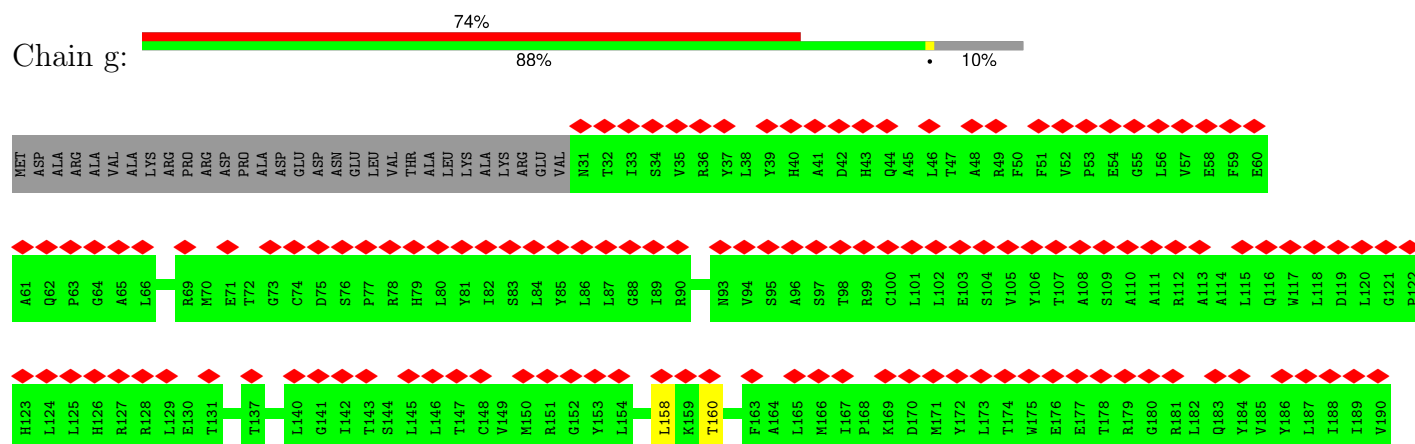
- Molecule 3: Small capsomere-interacting protein

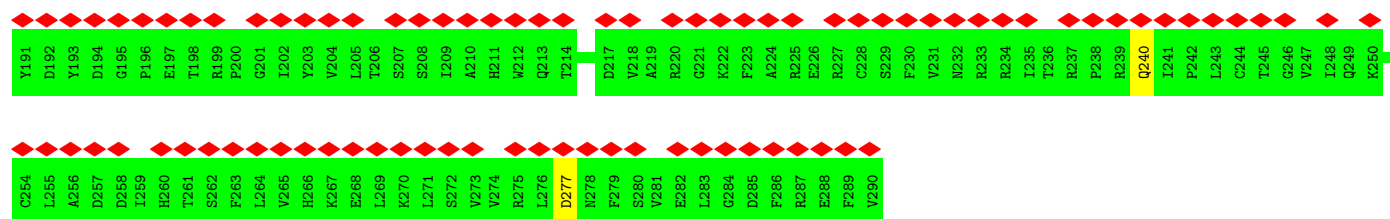


- Molecule 3: Small capsomere-interacting protein



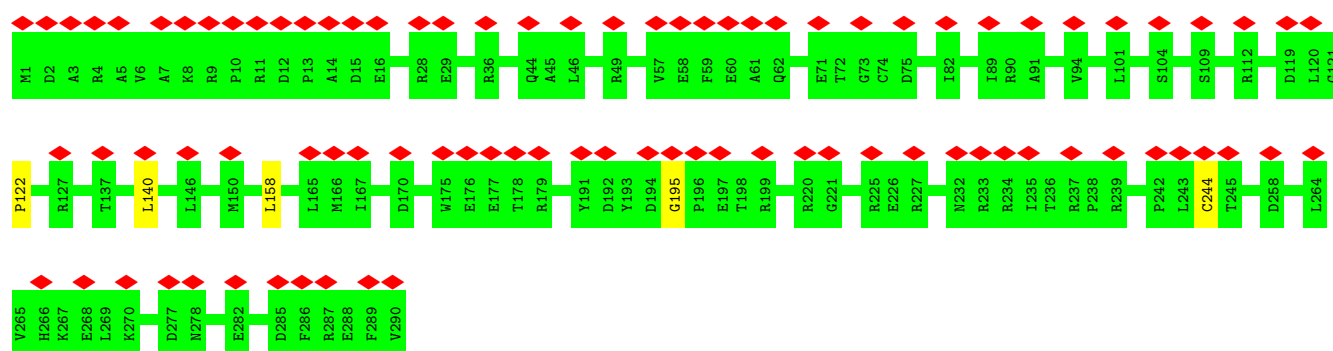
- Molecule 4: Triplex capsid protein 1





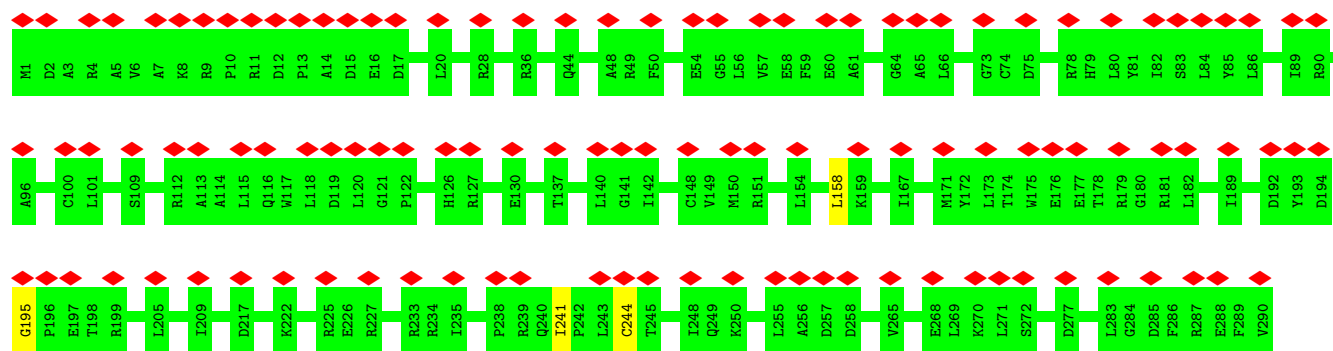
• Molecule 4: Triplex capsid protein 1

Chain j: 30% 98%



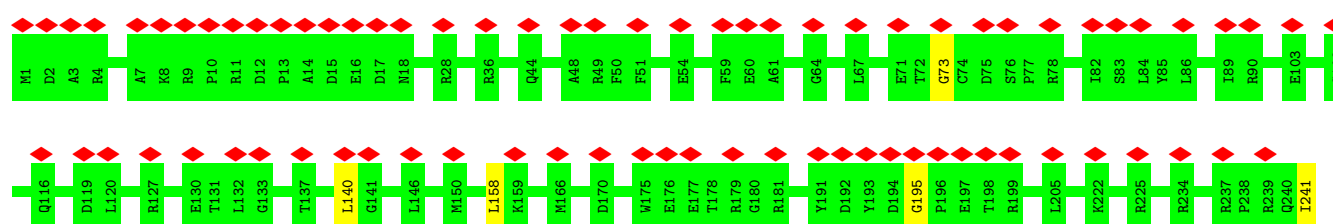
• Molecule 4: Triplex capsid protein 1

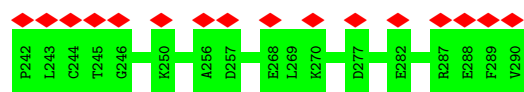
Chain m: 39% 99%



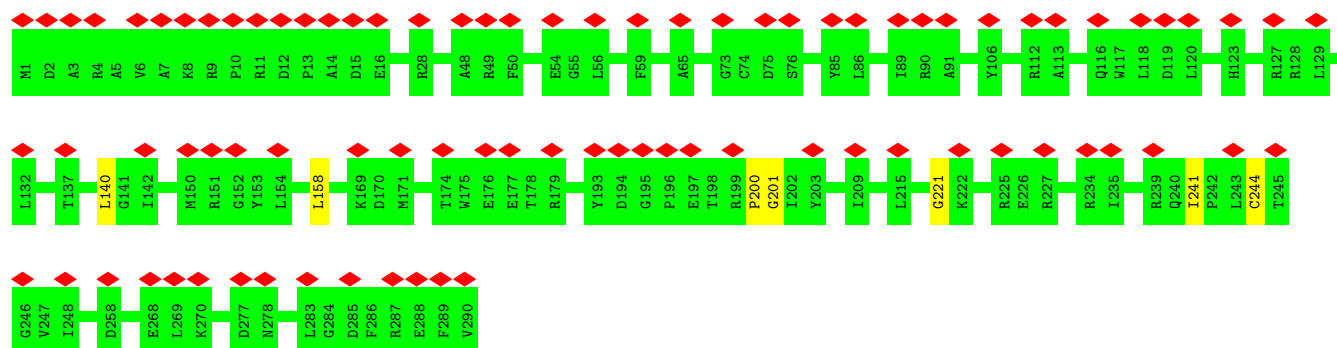
• Molecule 4: Triplex capsid protein 1

Chain p: 32% 98%

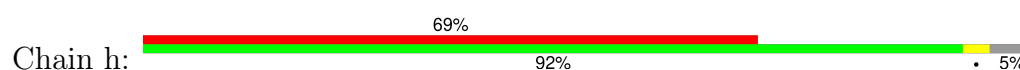




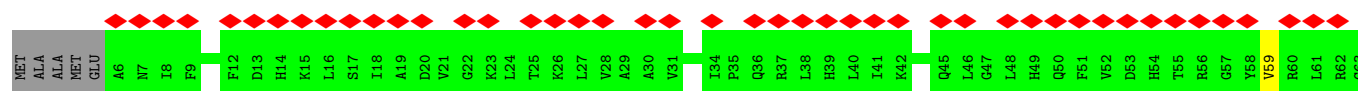
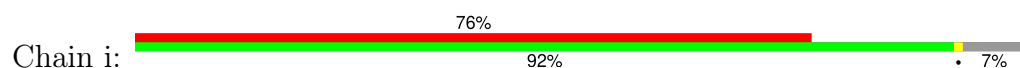
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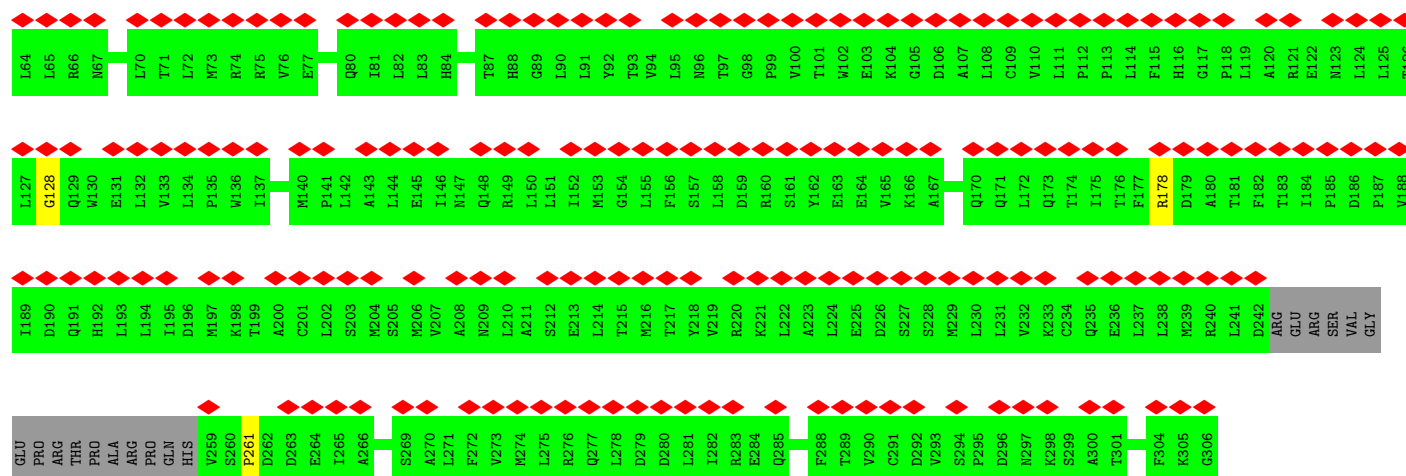


• Molecule 5: Triplex capsid protein 2



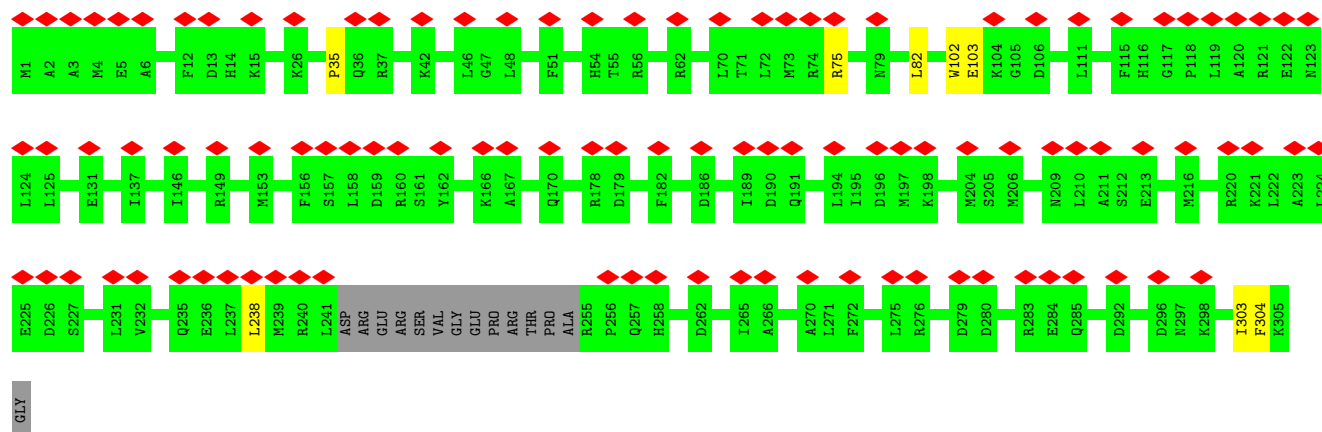
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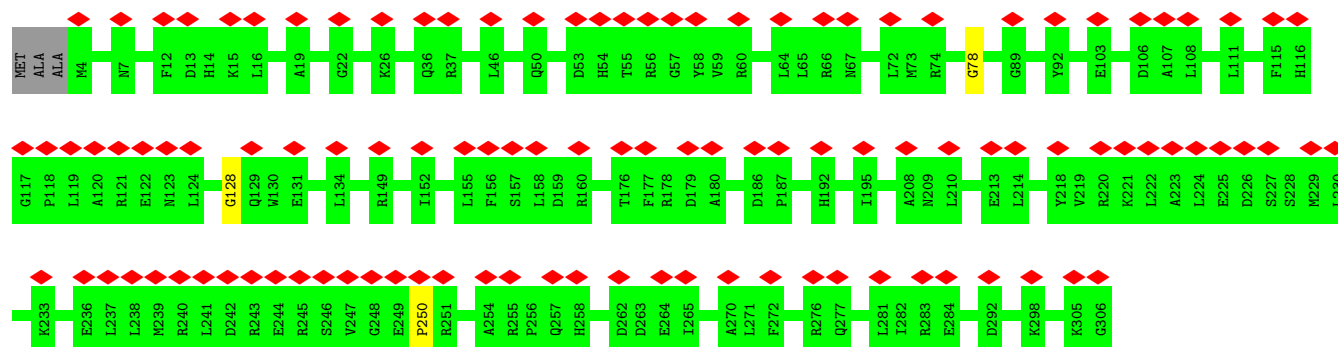
• Molecule 5: Triplex capsid protein 2

Chain k: 34% 93% 5%



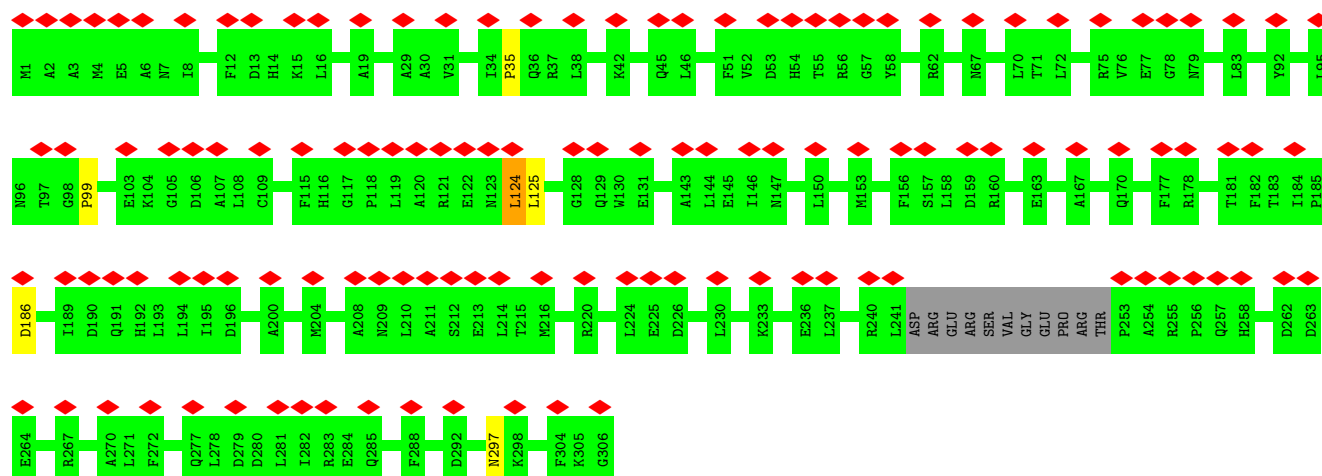
• Molecule 5: Triplex capsid protein 2

Chain l: 36% 98% 2%



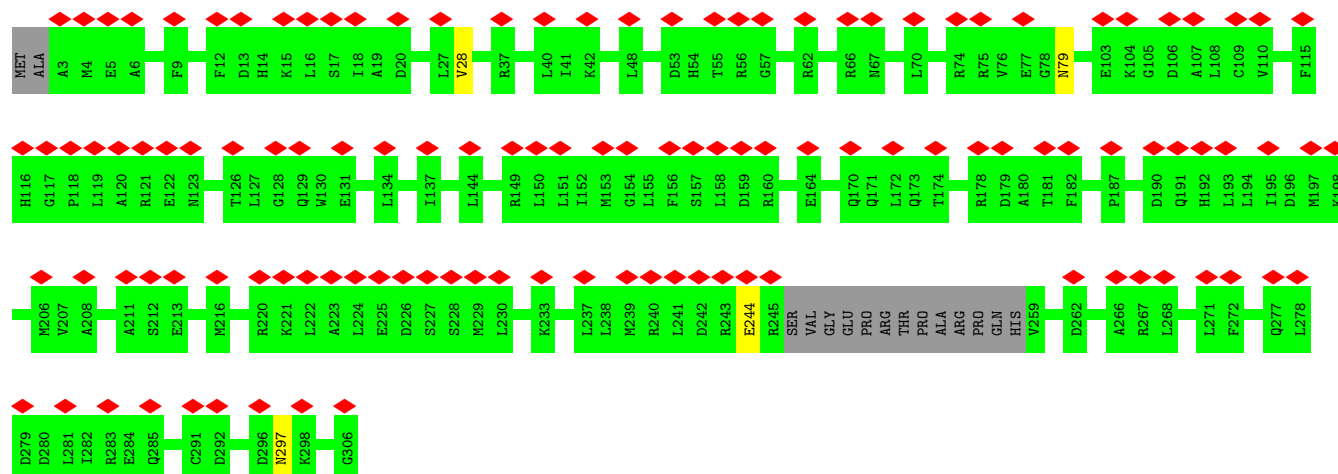
• Molecule 5: Triplex capsid protein 2

Chain n: 41% 94% 5%



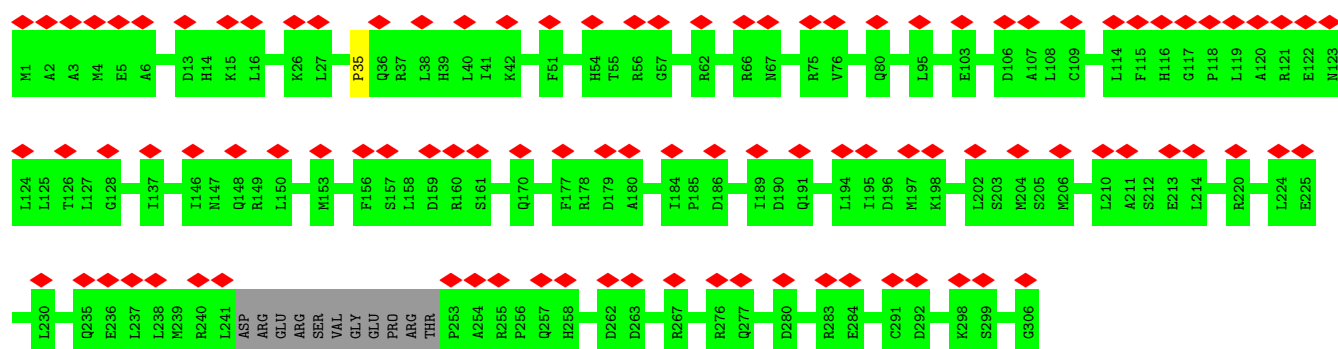
• Molecule 5: Triplex capsid protein 2

Chain o: 39% 94% 5%

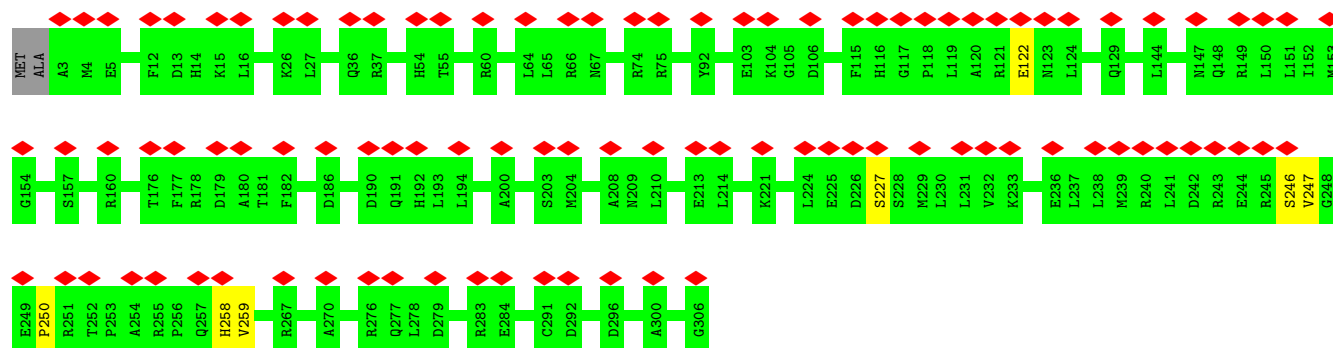


• Molecule 5: Triplex capsid protein 2

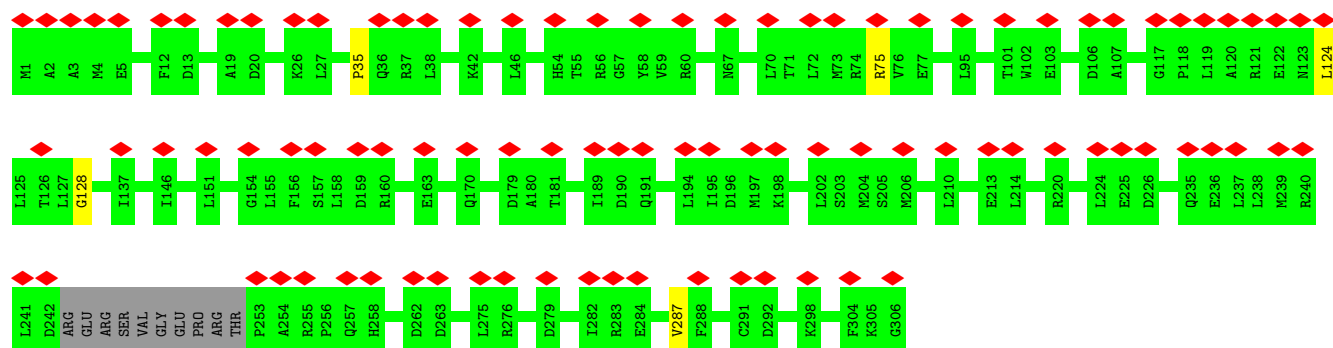
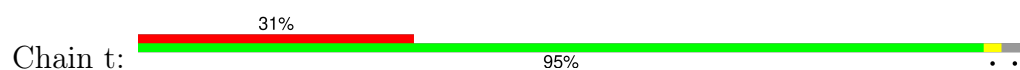
Chain q: 33% 96% 1%



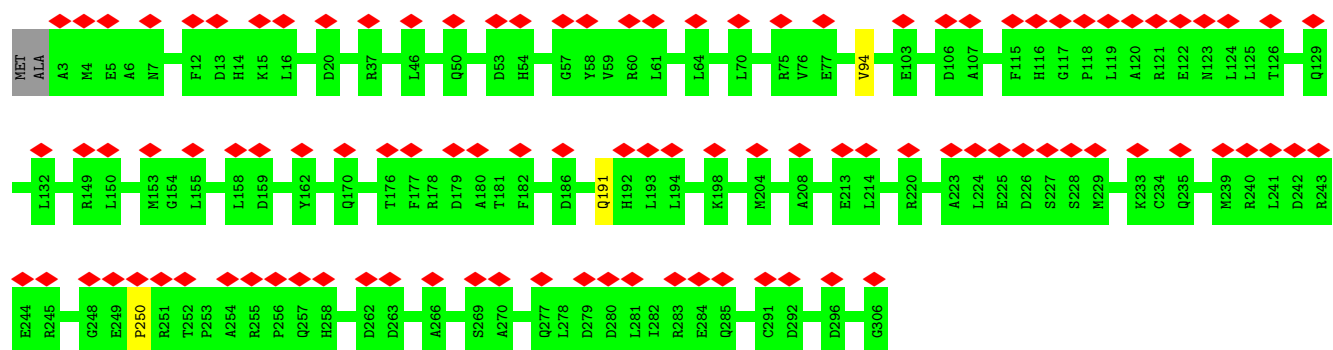
• Molecule 5: Triplex capsid protein 2



• 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	39600	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 ($e^-/\text{\AA}^2$)	2.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	1352.4, 1352.4, 1352.4	wwPDB
Map dimensions	840, 840, 840	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.61, 1.61, 1.61	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0	0.23	0/2366	0.37	0/3192
1	1	0.23	0/2366	0.38	0/3192
1	2	0.23	0/2366	0.38	0/3192
1	3	0.23	0/2366	0.37	0/3192
1	4	0.23	0/2366	0.38	0/3192
1	5	0.23	0/2366	0.37	0/3192
1	6	0.23	0/2366	0.37	0/3192
1	7	0.23	0/2366	0.38	0/3192
1	8	0.23	0/2366	0.37	0/3192
1	9	0.23	0/2366	0.38	0/3192
1	v	0.23	0/2366	0.38	0/3192
1	w	0.23	0/2366	0.38	0/3192
1	x	0.23	0/2366	0.38	0/3192
1	y	0.23	0/2366	0.37	0/3192
1	z	0.23	0/2366	0.37	0/3192
2	A	0.25	0/10780	0.44	0/14685
2	B	0.25	0/10824	0.44	0/14743
2	C	0.25	0/10942	0.44	1/14906 (0.0%)
2	D	0.25	0/10926	0.44	0/14884
2	E	0.25	0/10932	0.44	0/14892
2	F	0.25	0/10949	0.43	0/14916
2	G	0.25	0/10962	0.43	0/14933
2	H	0.25	0/10967	0.43	0/14940
2	I	0.25	0/10932	0.43	1/14892 (0.0%)
2	J	0.25	0/10835	0.43	1/14757 (0.0%)
2	K	0.25	0/10937	0.44	0/14899
2	L	0.25	0/10974	0.43	0/14950
2	M	0.25	0/10974	0.43	0/14950
2	N	0.25	0/10949	0.43	0/14916
2	O	0.25	0/10937	0.43	0/14899
2	P	0.25	0/10937	0.43	0/14899
3	Q	0.22	0/520	0.38	0/697
3	R	0.23	0/520	0.38	0/697
3	S	0.24	0/520	0.38	0/697

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	T	0.24	0/520	0.38	0/697
3	U	0.23	0/520	0.38	0/697
3	V	0.23	0/520	0.37	0/697
3	W	0.23	0/520	0.37	0/697
3	X	0.23	0/520	0.38	0/697
3	Y	0.23	0/520	0.37	0/697
3	Z	0.23	0/520	0.38	0/697
3	a	0.23	0/520	0.37	0/697
3	b	0.23	0/520	0.37	0/697
3	c	0.23	0/520	0.38	0/697
3	d	0.23	0/520	0.37	0/697
3	e	0.23	0/520	0.37	0/697
3	f	0.23	0/520	0.37	0/697
4	g	0.24	0/2138	0.44	0/2903
4	j	0.25	0/2374	0.43	0/3221
4	m	0.24	0/2374	0.43	0/3221
4	p	0.25	0/2374	0.43	0/3221
4	s	0.25	0/2374	0.43	0/3221
5	h	0.25	0/2361	0.44	0/3206
5	i	0.25	0/2300	0.46	0/3124
5	k	0.25	0/2361	0.43	0/3207
5	l	0.24	0/2453	0.43	0/3332
5	n	0.24	0/2379	0.45	1/3230 (0.0%)
5	o	0.24	0/2353	0.42	0/3193
5	q	0.24	0/2379	0.43	0/3230
5	r	0.24	0/2458	0.43	0/3339
5	t	0.25	0/2387	0.45	0/3241
5	u	0.24	0/2458	0.43	0/3339
All	All	0.25	0/254090	0.42	4/345321 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1367	LEU	CB-CG-CD2	-6.90	99.26	111.00
2	J	1367	LEU	CB-CG-CD1	-6.42	100.09	111.00
2	I	1367	LEU	CB-CG-CD2	-5.55	101.56	111.00
5	n	124	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	0	283/285 (99%)	274 (97%)	6 (2%)	3 (1%)	12	45
1	1	283/285 (99%)	267 (94%)	13 (5%)	3 (1%)	12	45
1	2	283/285 (99%)	267 (94%)	14 (5%)	2 (1%)	19	54
1	3	283/285 (99%)	266 (94%)	11 (4%)	6 (2%)	5	33
1	4	283/285 (99%)	271 (96%)	10 (4%)	2 (1%)	19	54
1	5	283/285 (99%)	272 (96%)	7 (2%)	4 (1%)	9	39
1	6	283/285 (99%)	271 (96%)	10 (4%)	2 (1%)	19	54
1	7	283/285 (99%)	267 (94%)	13 (5%)	3 (1%)	12	45
1	8	283/285 (99%)	275 (97%)	5 (2%)	3 (1%)	12	45
1	9	283/285 (99%)	271 (96%)	8 (3%)	4 (1%)	9	39
1	v	283/285 (99%)	262 (93%)	13 (5%)	8 (3%)	4	28
1	w	283/285 (99%)	269 (95%)	12 (4%)	2 (1%)	19	54
1	x	283/285 (99%)	264 (93%)	14 (5%)	5 (2%)	7	35
1	y	283/285 (99%)	270 (95%)	11 (4%)	2 (1%)	19	54
1	z	283/285 (99%)	272 (96%)	7 (2%)	4 (1%)	9	39
2	A	1321/1370 (96%)	1230 (93%)	78 (6%)	13 (1%)	13	46
2	B	1329/1370 (97%)	1226 (92%)	80 (6%)	23 (2%)	7	36
2	C	1345/1370 (98%)	1259 (94%)	71 (5%)	15 (1%)	12	45
2	D	1342/1370 (98%)	1233 (92%)	94 (7%)	15 (1%)	12	45
2	E	1343/1370 (98%)	1233 (92%)	90 (7%)	20 (2%)	8	39
2	F	1346/1370 (98%)	1242 (92%)	87 (6%)	17 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	1347/1370 (98%)	1250 (93%)	82 (6%)	15 (1%)	12	45
2	H	1348/1370 (98%)	1253 (93%)	86 (6%)	9 (1%)	19	54
2	I	1343/1370 (98%)	1243 (93%)	88 (7%)	12 (1%)	14	48
2	J	1329/1370 (97%)	1239 (93%)	76 (6%)	14 (1%)	12	45
2	K	1344/1370 (98%)	1249 (93%)	87 (6%)	8 (1%)	22	57
2	L	1349/1370 (98%)	1259 (93%)	77 (6%)	13 (1%)	13	46
2	M	1349/1370 (98%)	1250 (93%)	89 (7%)	10 (1%)	19	54
2	N	1346/1370 (98%)	1256 (93%)	81 (6%)	9 (1%)	19	54
2	O	1344/1370 (98%)	1243 (92%)	84 (6%)	17 (1%)	10	41
2	P	1344/1370 (98%)	1249 (93%)	81 (6%)	14 (1%)	13	46
3	Q	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	R	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
3	S	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	T	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	U	61/75 (81%)	56 (92%)	5 (8%)	0	100	100
3	V	61/75 (81%)	56 (92%)	4 (7%)	1 (2%)	8	37
3	W	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	X	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
3	Y	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
3	Z	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	a	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
3	b	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	c	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
3	d	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
3	e	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
3	f	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
4	g	258/290 (89%)	234 (91%)	21 (8%)	3 (1%)	11	43
4	j	288/290 (99%)	267 (93%)	17 (6%)	4 (1%)	9	39
4	m	288/290 (99%)	272 (94%)	14 (5%)	2 (1%)	19	54
4	p	288/290 (99%)	269 (93%)	16 (6%)	3 (1%)	13	46
4	s	288/290 (99%)	266 (92%)	17 (6%)	5 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	h	288/306 (94%)	260 (90%)	21 (7%)	7 (2%)	5	30
5	i	281/306 (92%)	257 (92%)	20 (7%)	4 (1%)	9	39
5	k	288/306 (94%)	268 (93%)	14 (5%)	6 (2%)	5	33
5	l	301/306 (98%)	274 (91%)	24 (8%)	3 (1%)	13	46
5	n	291/306 (95%)	271 (93%)	15 (5%)	5 (2%)	7	36
5	o	287/306 (94%)	266 (93%)	18 (6%)	3 (1%)	13	46
5	q	291/306 (95%)	279 (96%)	11 (4%)	1 (0%)	37	70
5	r	302/306 (99%)	275 (91%)	21 (7%)	6 (2%)	6	33
5	t	292/306 (95%)	269 (92%)	19 (6%)	4 (1%)	9	39
5	u	302/306 (99%)	275 (91%)	24 (8%)	3 (1%)	13	46
All	All	31023/31905 (97%)	28879 (93%)	1807 (6%)	337 (1%)	15	45

5 of 337 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	183	PRO
2	A	694	ASN
2	A	805	LYS
2	B	203	ALA
2	B	844	ASP

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	0	256/257 (100%)	256 (100%)	0	100	100
1	1	256/257 (100%)	256 (100%)	0	100	100
1	2	256/257 (100%)	256 (100%)	0	100	100
1	3	256/257 (100%)	256 (100%)	0	100	100
1	4	256/257 (100%)	256 (100%)	0	100	100
1	5	256/257 (100%)	256 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	256/257 (100%)	256 (100%)	0	100	100
1	7	256/257 (100%)	255 (100%)	1 (0%)	89	91
1	8	256/257 (100%)	256 (100%)	0	100	100
1	9	256/257 (100%)	256 (100%)	0	100	100
1	v	256/257 (100%)	256 (100%)	0	100	100
1	w	256/257 (100%)	256 (100%)	0	100	100
1	x	256/257 (100%)	256 (100%)	0	100	100
1	y	256/257 (100%)	256 (100%)	0	100	100
1	z	256/257 (100%)	256 (100%)	0	100	100
2	A	1156/1192 (97%)	1153 (100%)	3 (0%)	91	92
2	B	1162/1192 (98%)	1158 (100%)	4 (0%)	91	92
2	C	1174/1192 (98%)	1171 (100%)	3 (0%)	91	92
2	D	1173/1192 (98%)	1167 (100%)	6 (0%)	86	90
2	E	1174/1192 (98%)	1166 (99%)	8 (1%)	81	86
2	F	1175/1192 (99%)	1170 (100%)	5 (0%)	89	91
2	G	1177/1192 (99%)	1175 (100%)	2 (0%)	92	94
2	H	1177/1192 (99%)	1173 (100%)	4 (0%)	91	92
2	I	1174/1192 (98%)	1171 (100%)	3 (0%)	91	92
2	J	1161/1192 (97%)	1156 (100%)	5 (0%)	89	91
2	K	1174/1192 (98%)	1170 (100%)	4 (0%)	91	92
2	L	1178/1192 (99%)	1176 (100%)	2 (0%)	92	94
2	M	1178/1192 (99%)	1176 (100%)	2 (0%)	92	94
2	N	1175/1192 (99%)	1170 (100%)	5 (0%)	89	91
2	O	1174/1192 (98%)	1170 (100%)	4 (0%)	91	92
2	P	1174/1192 (98%)	1170 (100%)	4 (0%)	91	92
3	Q	59/68 (87%)	59 (100%)	0	100	100
3	R	59/68 (87%)	59 (100%)	0	100	100
3	S	59/68 (87%)	59 (100%)	0	100	100
3	T	59/68 (87%)	59 (100%)	0	100	100
3	U	59/68 (87%)	59 (100%)	0	100	100
3	V	59/68 (87%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	W	59/68 (87%)	59 (100%)	0	100	100
3	X	59/68 (87%)	59 (100%)	0	100	100
3	Y	59/68 (87%)	58 (98%)	1 (2%)	56	72
3	Z	59/68 (87%)	59 (100%)	0	100	100
3	a	59/68 (87%)	59 (100%)	0	100	100
3	b	59/68 (87%)	58 (98%)	1 (2%)	56	72
3	c	59/68 (87%)	59 (100%)	0	100	100
3	d	59/68 (87%)	59 (100%)	0	100	100
3	e	59/68 (87%)	59 (100%)	0	100	100
3	f	59/68 (87%)	59 (100%)	0	100	100
4	g	228/252 (90%)	227 (100%)	1 (0%)	89	91
4	j	252/252 (100%)	251 (100%)	1 (0%)	89	91
4	m	252/252 (100%)	250 (99%)	2 (1%)	79	84
4	p	252/252 (100%)	250 (99%)	2 (1%)	79	84
4	s	252/252 (100%)	250 (99%)	2 (1%)	79	84
5	h	262/273 (96%)	260 (99%)	2 (1%)	79	84
5	i	256/273 (94%)	256 (100%)	0	100	100
5	k	262/273 (96%)	260 (99%)	2 (1%)	79	84
5	l	272/273 (100%)	272 (100%)	0	100	100
5	n	263/273 (96%)	262 (100%)	1 (0%)	89	91
5	o	261/273 (96%)	260 (100%)	1 (0%)	89	91
5	q	263/273 (96%)	263 (100%)	0	100	100
5	r	272/273 (100%)	271 (100%)	1 (0%)	89	91
5	t	264/273 (97%)	263 (100%)	1 (0%)	89	91
5	u	272/273 (100%)	272 (100%)	0	100	100
All	All	27423/28005 (98%)	27340 (100%)	83 (0%)	90	92

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	207	LEU
5	k	82	LEU
2	O	431	LEU

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Mol	Chain	Res	Type
3	Y	73	THR
5	n	297	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	749	HIS
2	L	1235	GLN
5	t	192	HIS
2	K	901	HIS
2	L	618	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.

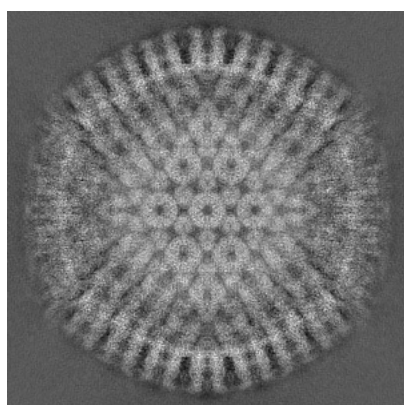
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8703. These allow visual inspection of the internal detail of the map and identification of artifacts.

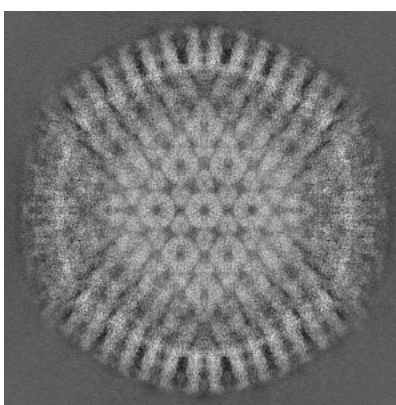
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

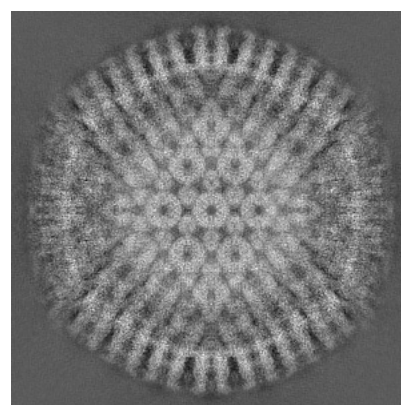
6.1.1 Primary map



X



Y

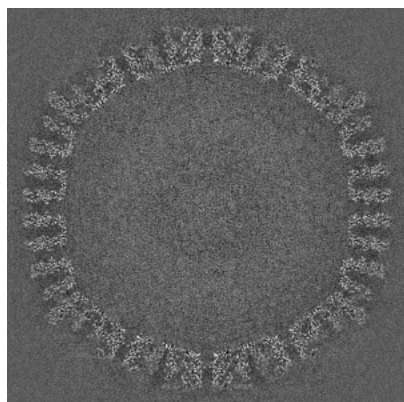


Z

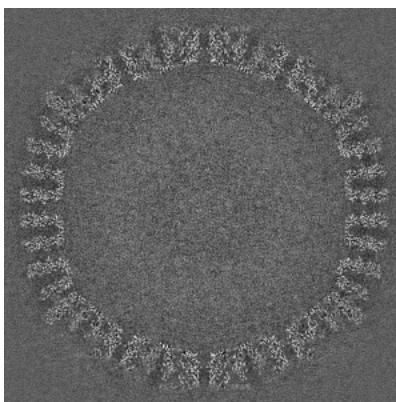
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

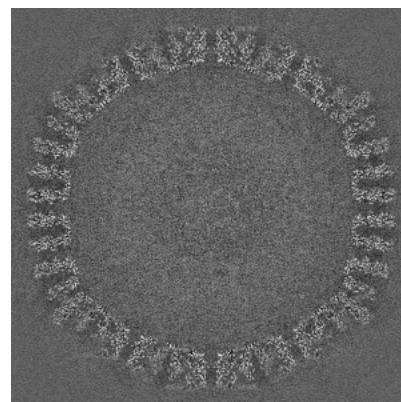
6.2.1 Primary map



X Index: 420



Y Index: 420

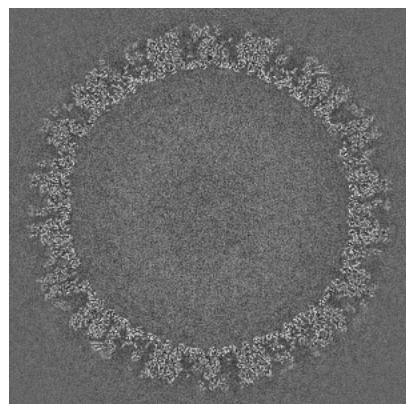


Z Index: 420

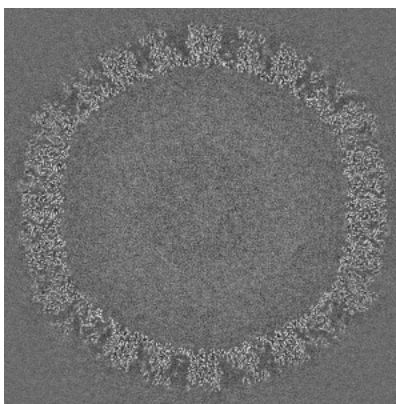
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

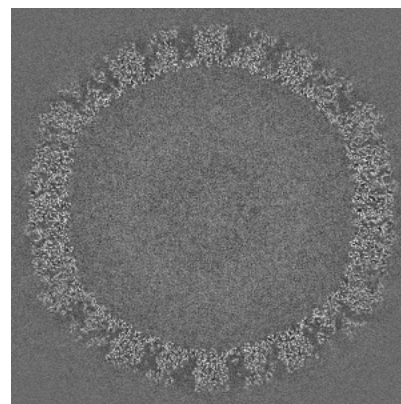
6.3.1 Primary map



X Index: 352



Y Index: 401

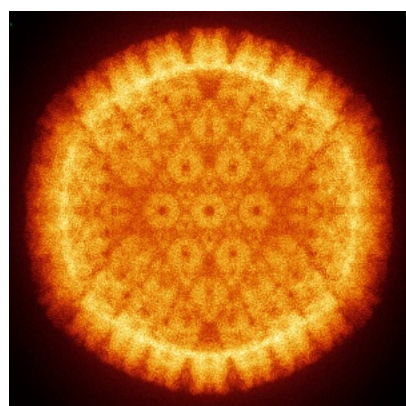


Z Index: 439

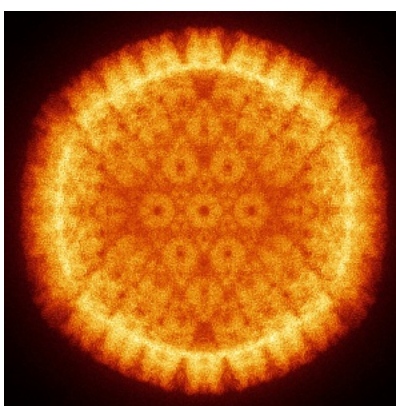
The images above show the largest variance slices of the map in three orthogonal directions.

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

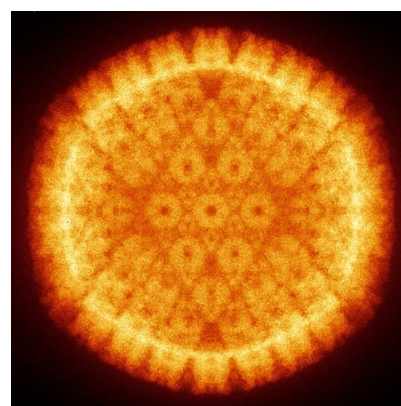
6.4.1 Primary map



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

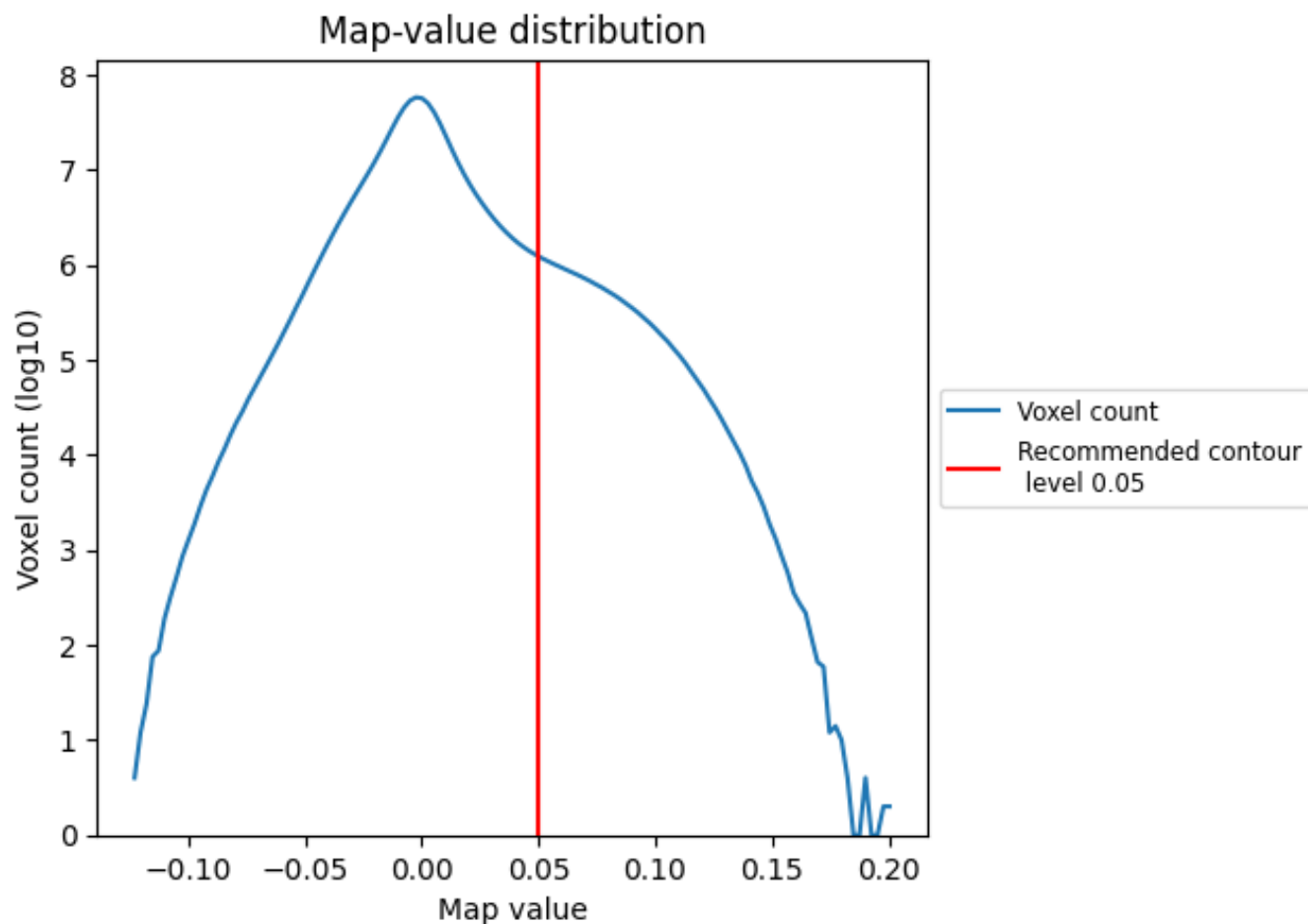
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

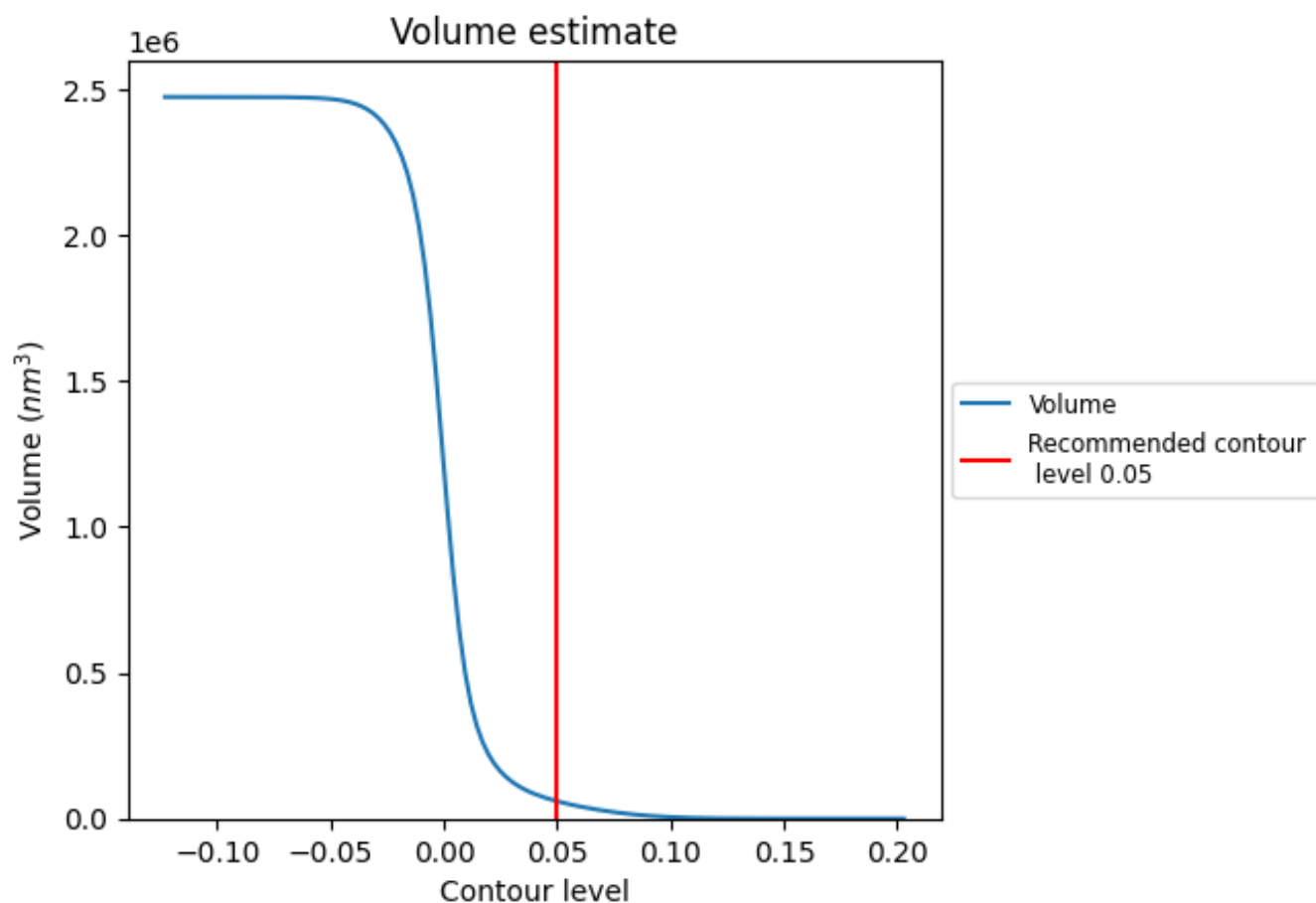
This section contains the results of statistical analysis of the map.

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.

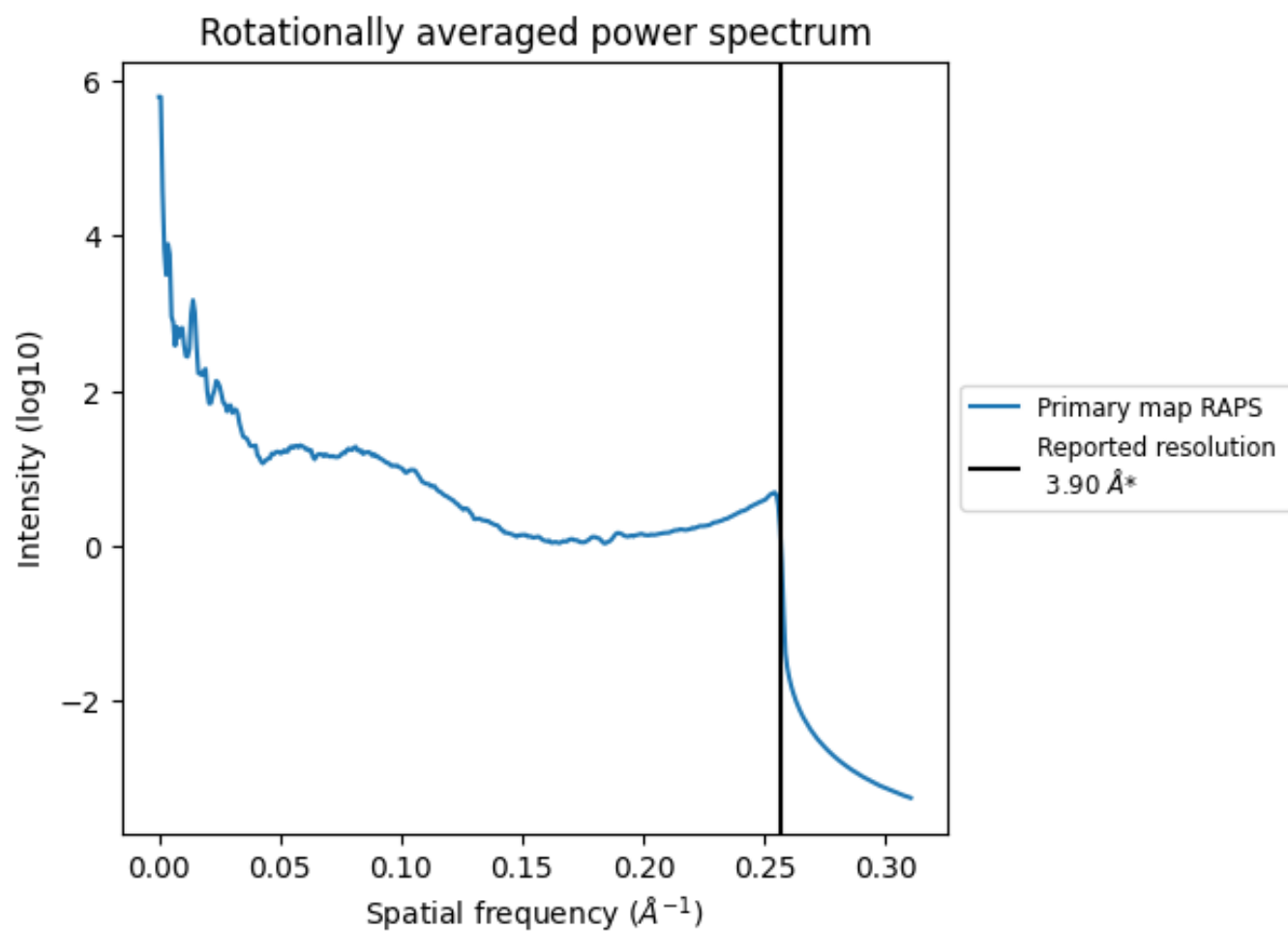
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59607 nm³; this corresponds to an approximate mass of 53844 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 0.256 Å⁻¹

8 Fourier-Shell correlation

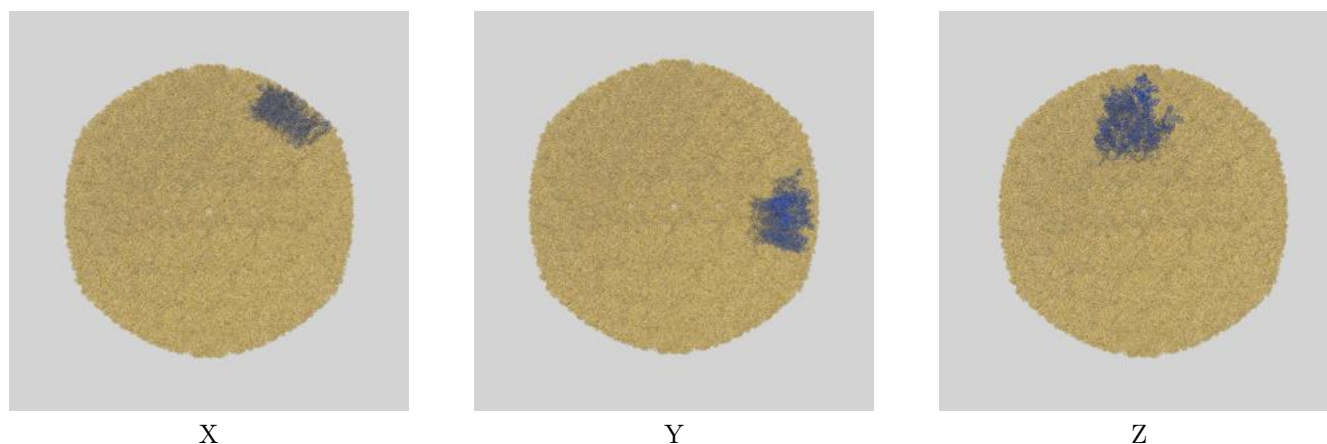
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

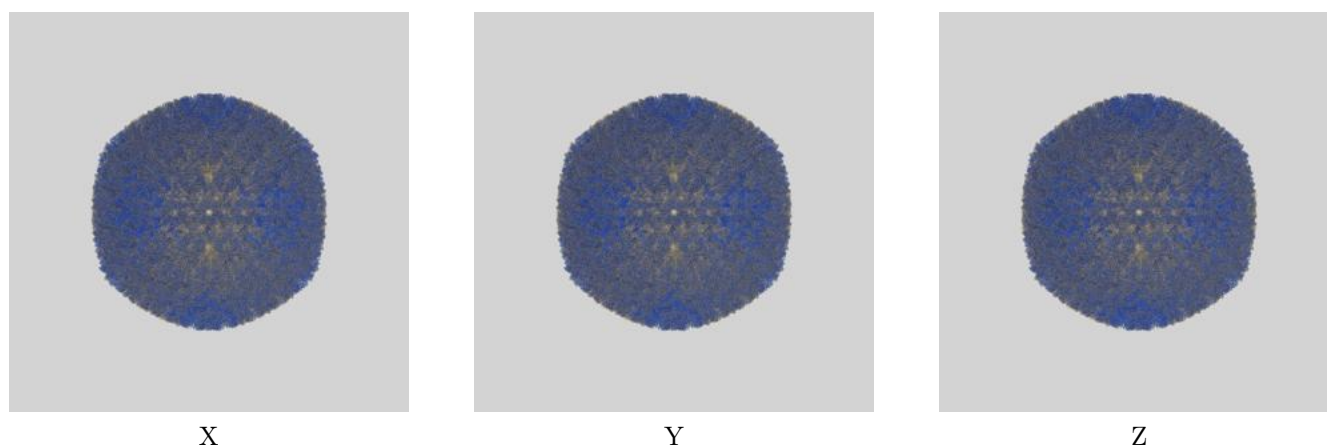
This section contains information regarding the fit between EMDB map EMD-8703 and PDB model 5VKU. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

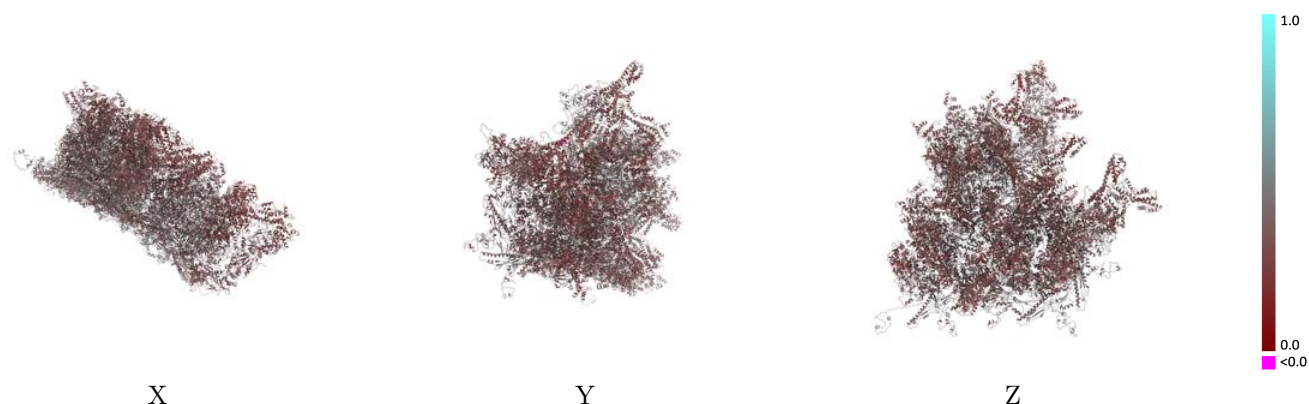


9.1.2 Map-model assembly overlay [i](#)



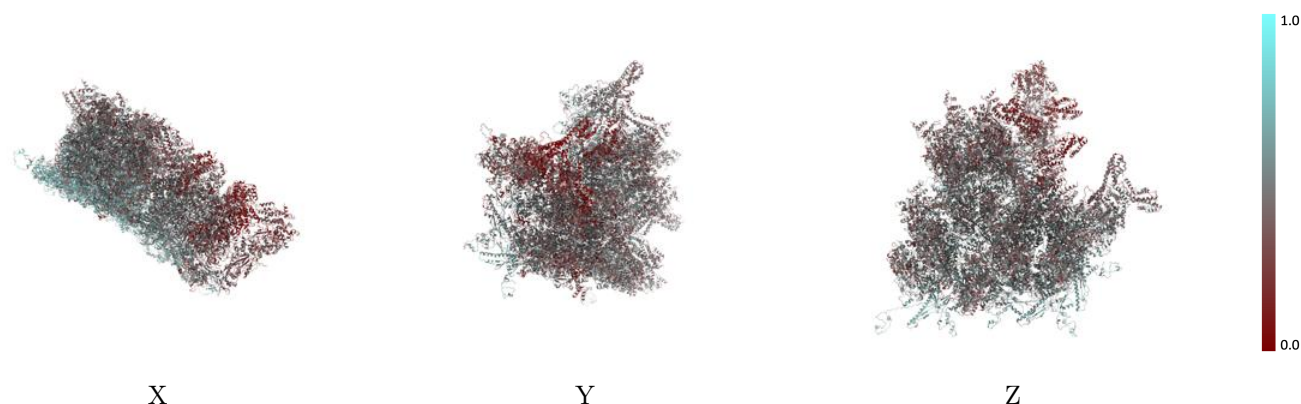
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



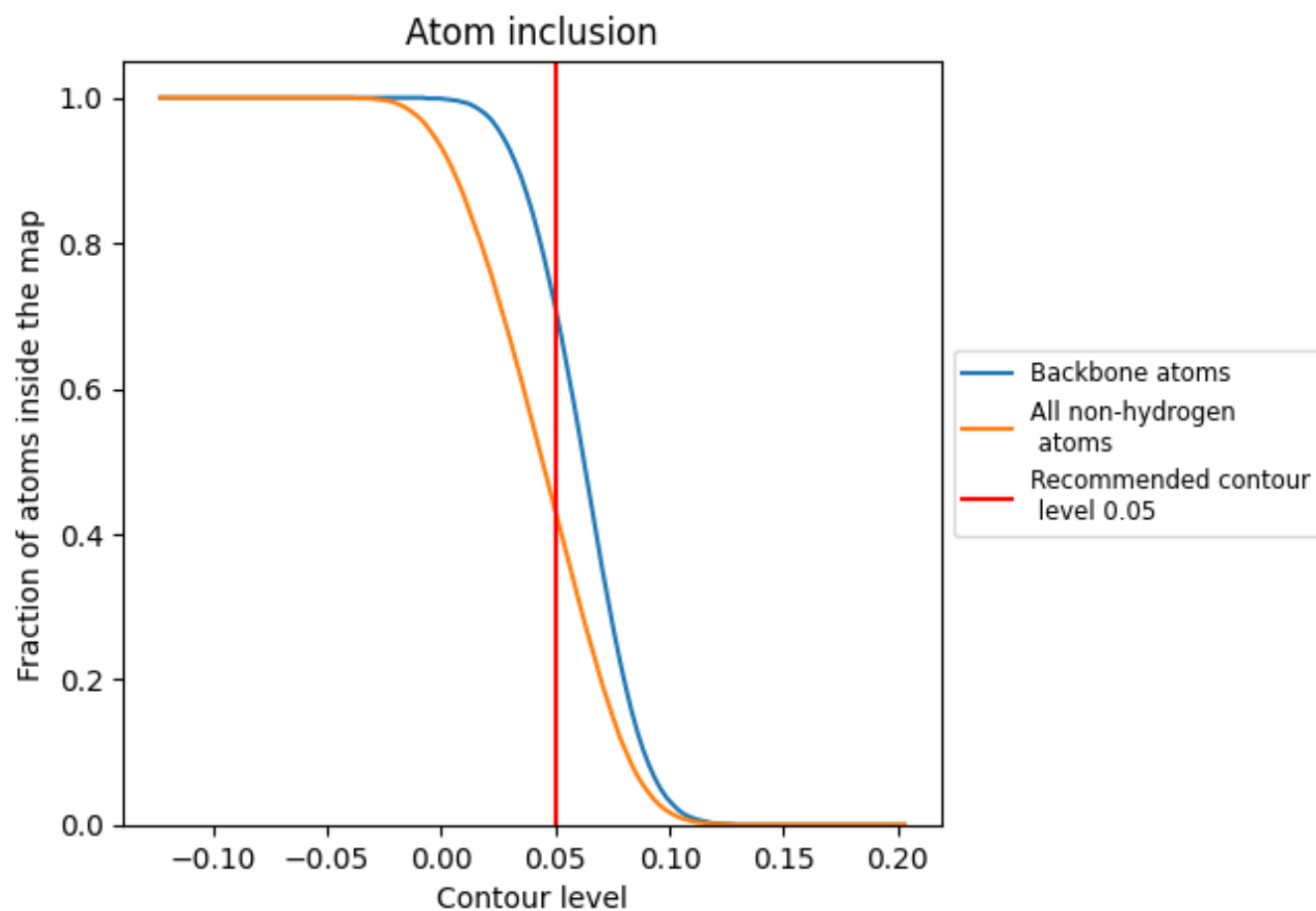
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

























































The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4310	0.3470
0	0.3760	0.3020
1	0.3730	0.3070
2	0.1320	0.2890
3	0.2690	0.2770
4	0.4040	0.3190
5	0.3450	0.2850
6	0.3680	0.3050
7	0.4100	0.3090
8	0.3800	0.3030
9	0.3770	0.3140
A	0.3050	0.3280
B	0.4120	0.3430
C	0.4470	0.3540
D	0.4700	0.3600
E	0.4720	0.3630
F	0.4490	0.3580
G	0.4130	0.3450
H	0.4860	0.3590
I	0.4920	0.3670
J	0.4900	0.3660
K	0.4940	0.3690
L	0.4950	0.3710
M	0.4800	0.3610
N	0.4910	0.3670
O	0.4950	0.3670
P	0.4940	0.3650
Q	0.1730	0.2680
R	0.2630	0.2730
S	0.3050	0.2750
T	0.3330	0.2920
U	0.3330	0.2860
V	0.3250	0.2910
W	0.2850	0.2920
X	0.3710	0.2930



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Chain	Atom inclusion	Q-score
Y	 0.3760	 0.3030
Z	 0.3920	 0.3170
a	 0.3730	 0.3000
b	 0.3760	 0.2850
c	 0.3590	 0.2890
d	 0.3880	 0.3160
e	 0.3800	 0.3000
f	 0.3670	 0.2860
g	 0.2420	 0.3340
h	 0.2850	 0.3180
i	 0.2500	 0.3320
j	 0.4910	 0.3740
k	 0.4690	 0.3600
l	 0.4500	 0.3620
m	 0.4580	 0.3500
n	 0.4450	 0.3520
o	 0.4500	 0.3530
p	 0.4770	 0.3570
q	 0.4690	 0.3630
r	 0.4660	 0.3550
s	 0.4890	 0.3710
t	 0.4800	 0.3690
u	 0.4590	 0.3580
v	 0.0800	 0.2740
w	 0.0930	 0.2480
x	 0.2160	 0.2720
y	 0.3910	 0.3270
z	 0.3850	 0.3050