



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 05:01 AM JST

PDB ID : 8H2I
EMDB ID : EMD-34438
Title : Near-atomic structure of five-fold averaged PBCV-1 capsid
Authors : Shao, Q.; Agarkova, I.V.; Noel, E.A.; Dunigan, D.D.; Liu, Y.; Wang, A.; Guo, M.; Xie, L.; Zhao, X.; Rossmann, M.G.; Van Etten, J.L.; Klose, T.; Fang, Q.
Deposited on : 2022-10-06
Resolution : 3.80 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

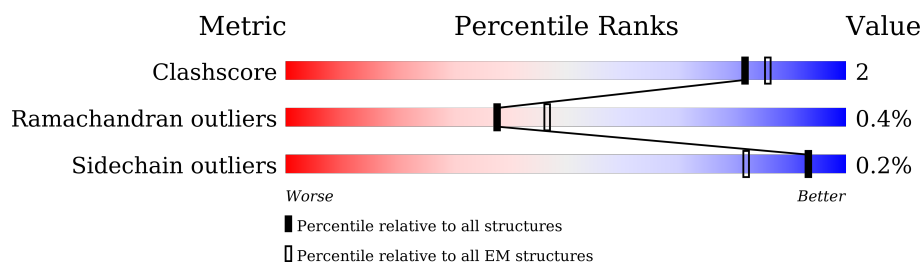
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	aA	437	<div> <div>85%</div> <div>99%</div> </div>
1	aB	437	<div> <div>81%</div> <div>100%</div> </div>
1	aC	437	<div> <div>78%</div> <div>100%</div> </div>
1	aD	437	<div> <div>78%</div> <div>99%</div> <div>.</div> </div>
1	aE	437	<div> <div>52%</div> <div>100%</div> </div>
1	aF	437	<div> <div>44%</div> <div>99%</div> <div>.</div> </div>
1	aG	437	<div> <div>59%</div> <div>99%</div> </div>
1	aH	437	<div> <div>38%</div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	aI	437	40% 99%
1	aJ	437	46% 100%
1	aK	437	54% 99%
1	aL	437	60% 99%
1	aM	437	62% 100%
1	aN	437	58% 99%
1	aO	437	63% 100%
1	aP	437	57% 100%
1	aQ	437	68% 99%
1	aR	437	71% 99%
1	aS	437	65% 100%
1	aT	437	62% 99%
1	aU	437	56% 100%
1	aV	437	57% 99%
1	aW	437	70% 100%
1	aX	437	70% 100%
1	aY	437	72% 100%
1	aZ	437	66% 100%
1	aa	437	45% 99%
1	ab	437	45% 99%
1	ac	437	42% 100%
1	ad	437	43% 99%
1	ae	437	42% 100%
1	af	437	47% 100%
1	ag	437	45% 100%

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Mol	Chain	Length	Quality of chain
1	ah	437	37% 99%
1	ai	437	44% 100%
1	aj	437	75% 100%
1	ak	437	62% 99%
1	al	437	78% 99%
1	am	437	41% 100%
1	an	437	41% 99%
1	ao	437	41% 99%
1	ap	437	38% 100%
1	aq	437	33% 100%
1	ar	437	31% 99%
1	as	437	44% 99%
1	at	437	58% 100%
1	au	437	51% 99%
1	av	437	69% 100%
1	aw	437	75% 100%
1	ax	437	65% 99%
1	ay	437	88% 100%
1	az	437	89% 99%
1	ba	437	57% 100%
1	bb	437	67% 99%
1	bc	437	58% 100%
1	bd	437	62% 99%
1	be	437	61% 100%
1	bf	437	55% 99%

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Mol	Chain	Length	Quality of chain
1	bg	437	58% 100%
1	bh	437	55% 100%
1	bi	437	62% 100%
1	bj	437	68% 100%
1	bk	437	61% 99%
1	bl	437	67% 99%
1	bm	437	66% 100%
1	bn	437	70% 99%
1	bo	437	68% 99%
1	bp	437	60% 100%
1	bq	437	68% 100%
1	br	437	48% 99%
1	bs	437	58% 100%
1	bt	437	56% 99%
2	bA	520	58% 98%
2	bB	520	79% 99%
2	bu	520	31% 98%
2	bv	520	36% 98%
2	bw	520	34% 99%
2	bx	520	42% 98%
2	by	520	49% 99%
2	bz	520	48% 97%
3	bC	486	61% 99%
4	bD	403	84% 99%
4	bF	403	77% 99%

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Mol	Chain	Length	Quality of chain
4	cX	403	68% 98% .
4	cZ	403	69% 98% .
4	dd	403	85% 98% .
4	df	403	85% 97% .
4	dj	403	75% 98% .
4	dk	403	76% 98% .
4	dl	403	70% 98% .
4	dp	403	73% 99% .
4	dr	403	71% 98% .
5	bE	401	74% 99% .
5	cY	401	83% 98% ..
5	de	401	86% 99% .
5	dq	401	77% 98% ..
6	bG	530	54% 95% 5%
7	bH	576	48% 73% 26%
8	bI	171	63% 82% 18%
8	bJ	171	63% 85% 14%
8	bK	171	51% 68% 32%
9	bL	181	29% 34% 65%
9	bM	181	31% 34% 65%
9	bN	181	29% 34% 66%
9	bO	181	32% 33% 66%
10	bP	146	77% 97% .
11	bQ	216	63% 73% 25%
12	bR	173	55% 92% 8%

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Mol	Chain	Length	Quality of chain
13	bS	210	
14	bT	207	
14	bU	207	
14	bV	207	
14	bW	207	
14	bX	207	
14	bY	207	
14	bZ	207	
14	ca	207	
14	cb	207	
14	cc	207	
14	cd	207	
14	ce	207	
15	cf	151	
16	cg	98	
17	ch	155	
18	ci	93	
19	cj	80	
19	ck	80	
19	cl	80	
19	cm	80	
20	cn	148	
20	co	148	
21	cA	378	
21	cB	378	

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Mol	Chain	Length	Quality of chain
21	cC	378	74%
21	cD	378	77%
21	cE	378	73%
21	cF	378	74%
21	cG	378	74%
21	cH	378	63%
21	cI	378	74%
21	cJ	378	71%
21	cK	378	74%
21	cL	378	75%
21	cM	378	73%
21	cN	378	77%
21	cp	378	77%
21	cq	378	75%
21	cr	378	76%
21	cs	378	73%
21	ct	378	76%
21	cu	378	74%
21	cv	378	72%
21	cw	378	71%
21	cx	378	63%
21	cy	378	72%
21	cz	378	77%
22	cO	1335	 98%
22	cQ	1335	 98%

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Mol	Chain	Length	Quality of chain
22	da	1335	98%
22	dc	1335	98%
22	dg	1335	98%
22	di	1335	98%
22	ds	1335	98%
22	du	1335	98%
23	cP	1369	97%
23	db	1369	98%
23	dh	1369	97%
23	dt	1369	97%
24	cR	400	77% 98%
24	cS	400	71% 98%
24	cT	400	75% 98%
25	cU	1343	97%
25	cV	1343	97%
25	cW	1343	97%
26	dm	1359	98%
26	dn	1359	98%
26	do	1359	98%

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 427569 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 (MCP).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aa	432	Total	C	N	O	S	0	0
			3374	2145	571	650	8		
1	ab	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ac	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ad	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ae	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	af	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ag	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ah	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ai	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aj	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ak	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	al	435	Total	C	N	O	S	0	0
			3387	2152	574	653	8		
1	am	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	an	435	Total	C	N	O	S	0	0
			3387	2152	574	653	8		
1	ao	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	ap	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aq	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ar	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	as	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	at	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	au	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	av	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aw	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ax	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	ay	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	az	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aA	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aB	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aC	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aD	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aE	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aF	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aG	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aH	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aI	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aJ	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aK	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aL	435	Total	C	N	O	S	0	0
			3387	2152	574	653	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	aM	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aN	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aO	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aP	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aQ	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aR	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aS	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aT	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aU	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aV	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aW	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aX	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aY	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aZ	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ba	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bb	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bc	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bd	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	be	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bf	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bg	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	bh	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bi	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bj	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bk	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bl	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bm	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bn	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	bo	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bp	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bq	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	br	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bs	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bt	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		

- Molecule 2 is a protein called MCPv1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	bu	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		
2	bv	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		
2	bw	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		
2	bx	514	Total	C	N	O	S	0	0
			4074	2611	677	775	11		
2	by	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		
2	bz	508	Total	C	N	O	S	0	0
			4030	2583	670	766	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	bA	516	Total	C	N	O	S	0	0
			4079	2612	679	777	11		
2	bB	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		

- Molecule 3 is a protein called MCPv2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	bC	485	Total	C	N	O	S	0	0
			3921	2518	645	742	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
bC	343	SER	GLY	variant	UNP M1I493

- Molecule 4 is a protein called MCPv3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	bF	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	cX	401	Total	C	N	O	S	0	0
			3165	2029	521	605	10		
4	cZ	401	Total	C	N	O	S	0	0
			3165	2029	521	605	10		
4	dd	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	df	401	Total	C	N	O	S	0	0
			3165	2029	521	605	10		
4	dj	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	dk	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	dl	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	dp	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	dr	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		

- Molecule 5 is a protein called MCPv4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	bE	397	Total	C	N	O	S	0	0
			3146	2021	513	601	11		
5	cY	397	Total	C	N	O	S	0	0
			3146	2021	513	601	11		
5	de	397	Total	C	N	O	S	0	0
			3146	2021	513	601	11		
5	dq	397	Total	C	N	O	S	0	0
			3146	2021	513	601	11		

- Molecule 6 is a protein called P1v1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	bG	504	Total	C	N	O	S	0	0
			3864	2454	633	771	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
bG	113	ASN	SER	variant	UNP M1I677
bG	348	ILE	VAL	variant	UNP M1I677
bG	364	SER	THR	variant	UNP M1I677

- Molecule 7 is a protein called P2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	bH	424	Total	C	N	O	S	0	0
			3258	2015	591	642	10		

- Molecule 8 is a protein called P3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	bI	141	Total	C	N	O	S	0	0
			1096	691	191	209	5		
8	bJ	147	Total	C	N	O	S	0	0
			1146	724	198	219	5		
8	bK	116	Total	C	N	O	S	0	0
			892	560	157	170	5		

- Molecule 9 is a protein called P4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	bL	63	Total	C	N	O	S	0	0
			526	340	88	97	1		
9	bM	63	Total	C	N	O	S	0	0
			526	340	88	97	1		
9	bN	62	Total	C	N	O	S	0	0
			519	336	87	95	1		
9	bO	62	Total	C	N	O	S	0	0
			519	336	87	95	1		

- Molecule 10 is a protein called P5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	bP	142	Total	C	N	O	S	0	0
			1126	724	192	208	2		

- Molecule 11 is a protein called P6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	bQ	162	Total	C	N	O	S	0	0
			1275	830	202	242	1		

- Molecule 12 is a protein called P8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	bR	159	Total	C	N	O	S	0	0
			1244	798	207	235	4		

- Molecule 13 is a protein called P9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	bS	191	Total	C	N	O	S	0	0
			1504	953	258	285	8		

- Molecule 14 is a protein called P11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	bT	48	Total	C	N	O	S	0	0
			373	237	65	69	2		
14	bU	54	Total	C	N	O	S	0	0
			424	273	70	79	2		
14	bV	53	Total	C	N	O	S	0	0
			416	269	68	77	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	bW	52	Total	C	N	O	S	0	0
			405	260	67	76	2		
14	bX	41	Total	C	N	O	S	0	0
			312	195	53	62	2		
14	bY	74	Total	C	N	O	S	0	0
			576	370	96	108	2		
14	bZ	52	Total	C	N	O	S	0	0
			405	260	67	76	2		
14	ca	52	Total	C	N	O	S	0	0
			405	260	67	76	2		
14	cb	52	Total	C	N	O	S	0	0
			405	260	67	76	2		
14	cc	84	Total	C	N	O	S	0	0
			646	415	107	122	2		
14	cd	75	Total	C	N	O	S	0	0
			583	375	97	109	2		
14	ce	72	Total	C	N	O	S	0	0
			560	359	93	106	2		

- Molecule 15 is a protein called P12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	cf	78	Total	C	N	O	S	0	0
			631	408	103	116	4		

- Molecule 16 is a protein called P13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	cg	66	Total	C	N	O	S	0	0
			521	333	89	96	3		

- Molecule 17 is a protein called P15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	ch	152	Total	C	N	O	S	0	0
			1288	838	212	233	5		

- Molecule 18 is a protein called P16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	ci	80	Total	C	N	O	S	0	0
			553	358	95	94	6		

- Molecule 19 is a protein called P17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	cj	59	Total	C	N	O	S	0	0
			463	295	76	90	2		
19	ck	57	Total	C	N	O	S	0	0
			455	293	76	84	2		
19	cl	55	Total	C	N	O	S	0	0
			431	275	71	82	3		
19	cm	63	Total	C	N	O	S	0	0
			503	320	86	95	2		

- Molecule 20 is a protein called P18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	cn	98	Total	C	N	O	S	0	0
			769	488	134	146	1		
20	co	95	Total	C	N	O	S	0	0
			733	470	123	139	1		

- Molecule 21 is a protein called P19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	cp	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cq	282	Total	C	N	O	S	0	0
			2212	1420	371	413	8		
21	cr	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cs	275	Total	C	N	O	S	0	0
			2159	1387	363	402	7		
21	ct	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cu	280	Total	C	N	O	S	0	0
			2199	1413	369	410	7		
21	cv	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cw	280	Total	C	N	O	S	0	0
			2199	1413	369	410	7		
21	cx	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cy	280	Total	C	N	O	S	0	0
			2199	1413	369	410	7		
21	cz	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	cA	279	Total	C	N	O	S	0	0
			2191	1409	367	408	7		
21	cB	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cC	279	Total	C	N	O	S	0	0
			2191	1409	367	408	7		
21	cD	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cE	280	Total	C	N	O	S	0	0
			2199	1413	369	410	7		
21	cF	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cG	282	Total	C	N	O	S	0	0
			2212	1420	371	413	8		
21	cH	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cI	279	Total	C	N	O	S	0	0
			2191	1409	367	408	7		
21	cJ	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cK	279	Total	C	N	O	S	0	0
			2191	1409	367	408	7		
21	cL	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cM	277	Total	C	N	O	S	0	0
			2173	1396	365	405	7		
21	cN	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		

- Molecule 22 is a protein called P20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	cO	30	Total	C	N	O	S	0	0
			218	142	35	39	2		
22	cQ	31	Total	C	N	O	S	0	0
			233	149	38	44	2		
22	da	32	Total	C	N	O	S	0	0
			228	144	37	45	2		
22	dc	28	Total	C	N	O	S	0	0
			209	134	34	39	2		
22	dg	32	Total	C	N	O	S	0	0
			241	153	40	46	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
22	di	29	Total	C	N	O	S	0	0
			211	137	32	40	2		
22	ds	32	Total	C	N	O	S	0	0
			238	152	40	44	2		
22	du	30	Total	C	N	O	S	0	0
			224	144	36	42	2		

- Molecule 23 is a protein called P21.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	cP	35	Total	C	N	O	0	0
			239	152	42	45		
23	db	30	Total	C	N	O	0	0
			200	127	36	37		
23	dh	35	Total	C	N	O	0	0
			249	157	45	47		
23	dt	35	Total	C	N	O	0	0
			236	147	44	45		

- Molecule 24 is a protein called MCPv5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	cR	399	Total	C	N	O	S	0	0
			3203	2060	518	611	14		
24	cS	399	Total	C	N	O	S	0	0
			3203	2060	518	611	14		
24	cT	399	Total	C	N	O	S	0	0
			3203	2060	518	611	14		

- Molecule 25 is a protein called P22.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	cU	43	Total	C	N	O	0	0
			311	203	51	57		
25	cV	43	Total	C	N	O	0	0
			305	201	50	54		
25	cW	43	Total	C	N	O	0	0
			308	202	51	55		

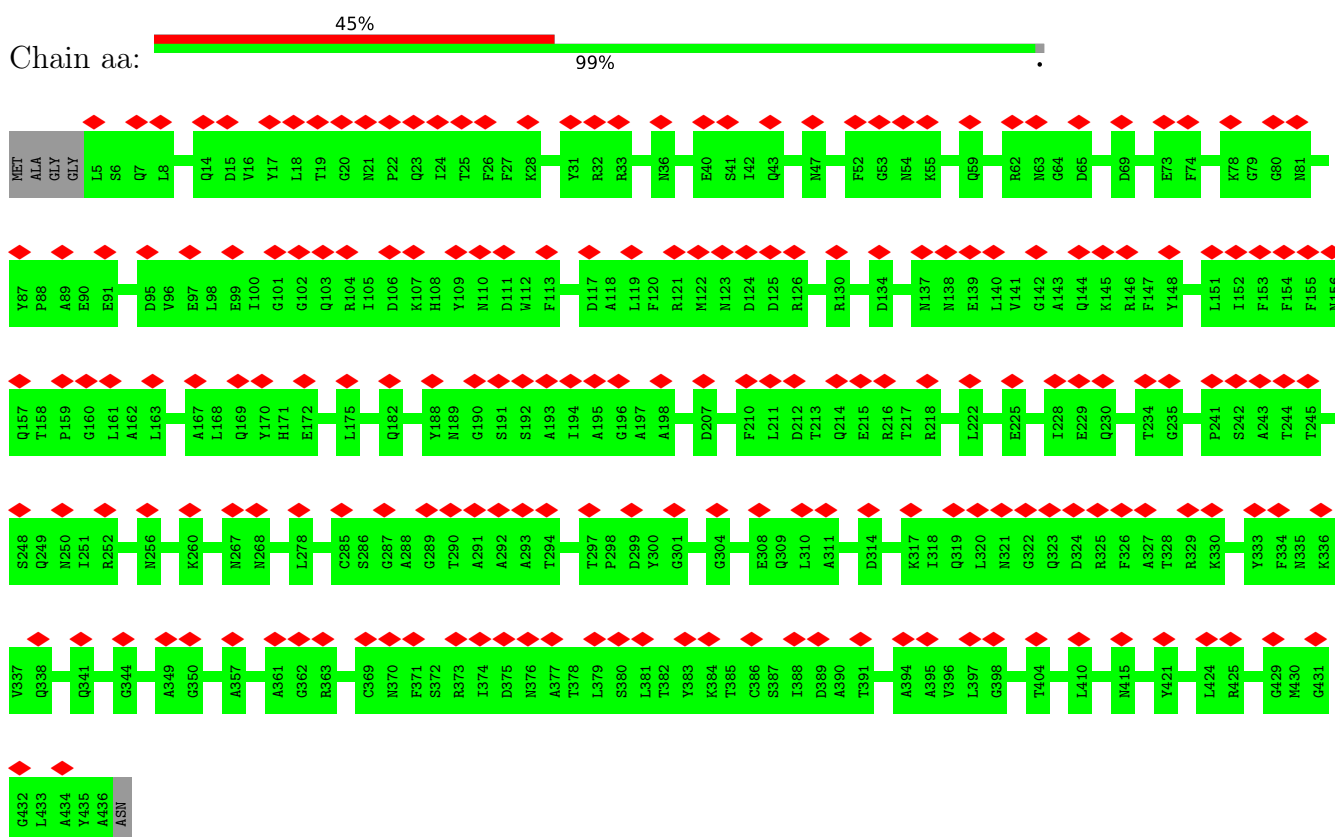
- Molecule 26 is a protein called P23.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	dm	25	Total 174	C 111	N 28	O 35	0	0
26	dn	25	Total 181	C 116	N 29	O 36	0	0
26	do	25	Total 182	C 121	N 28	O 33	0	0

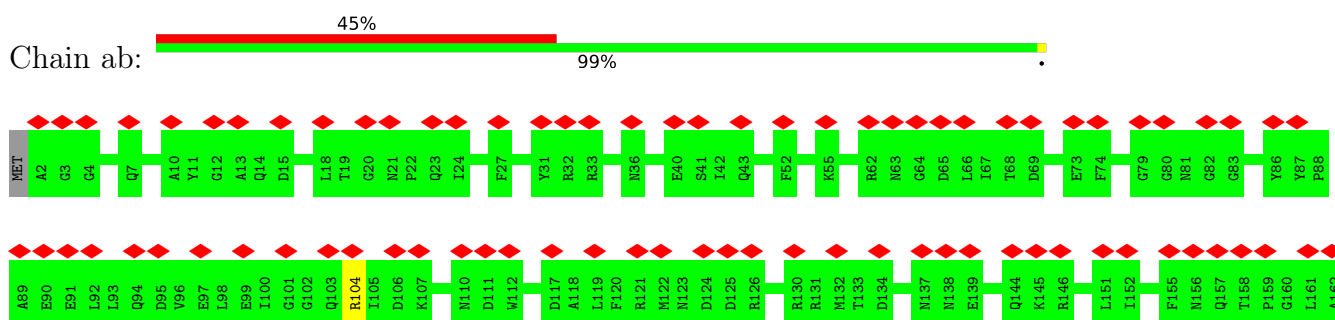
3 Residue-property plots [i](#)

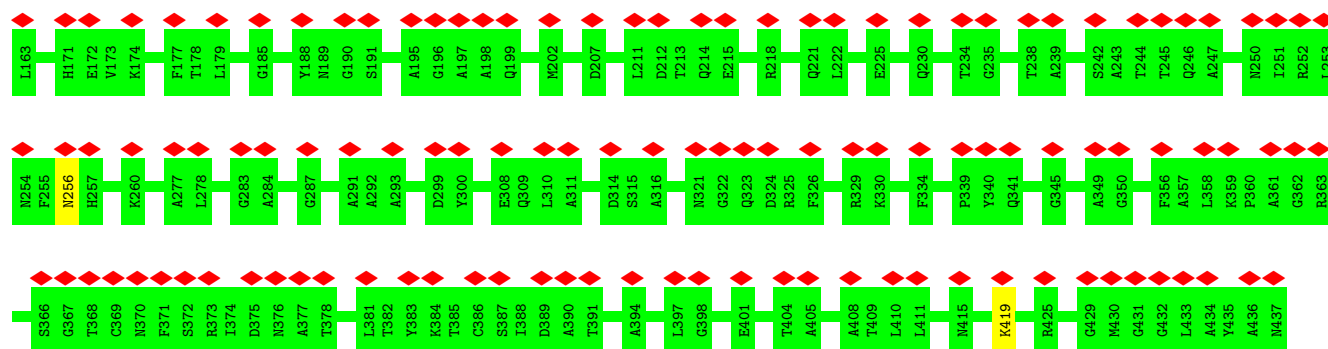
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Major capsid protein (MCP)

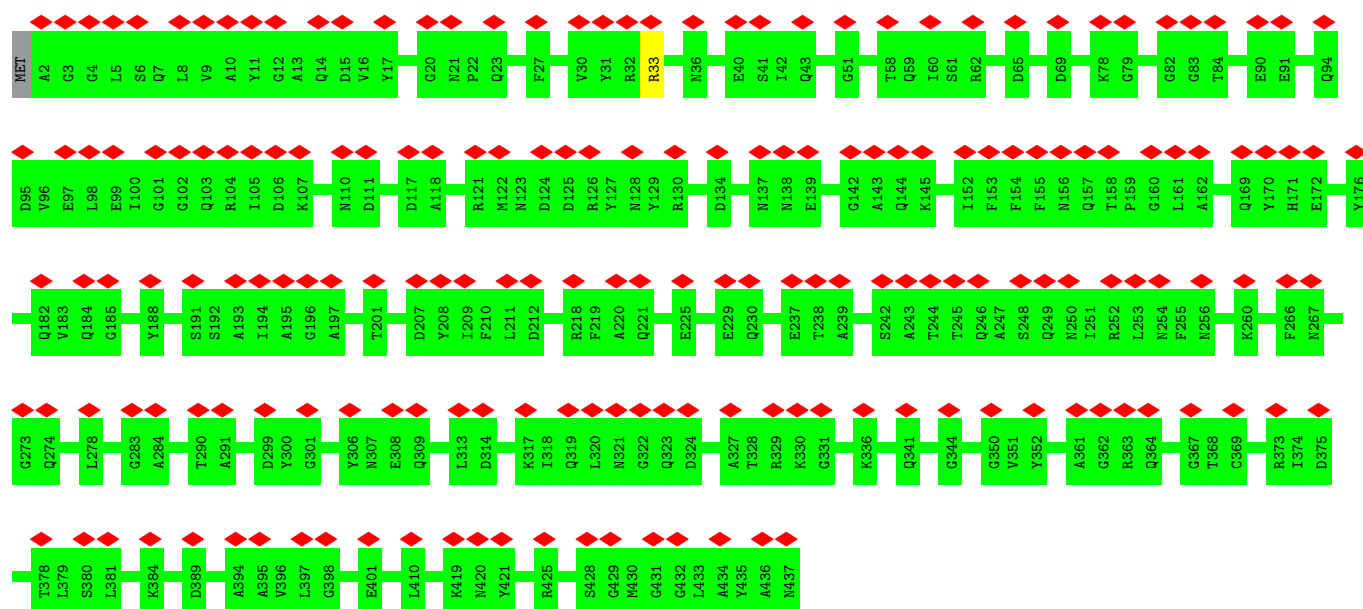
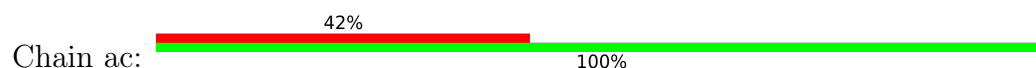


• Molecule 1: Major capsid protein (MCP)

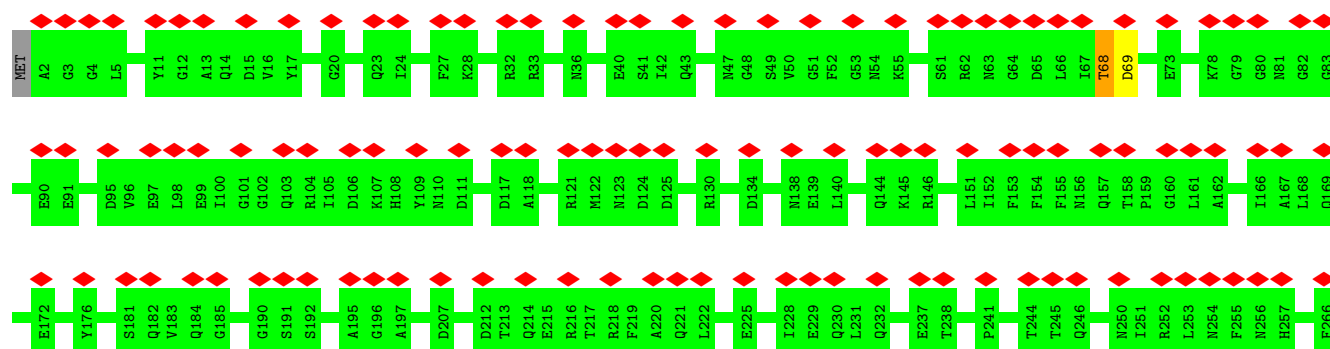
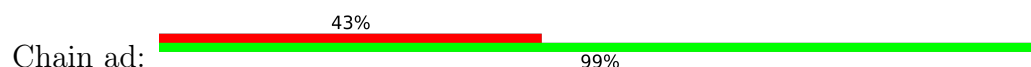


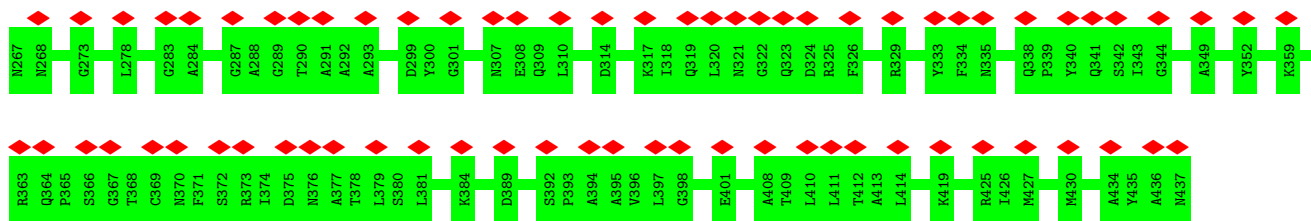


• Molecule 1: Major capsid protein (MCP)

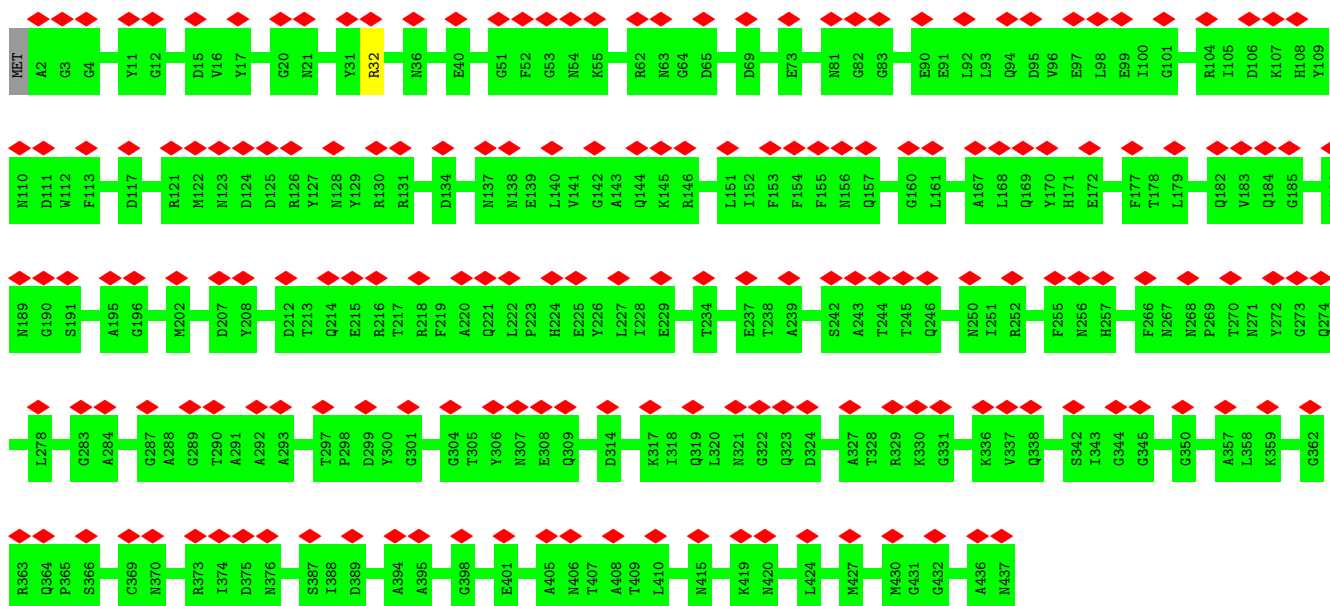
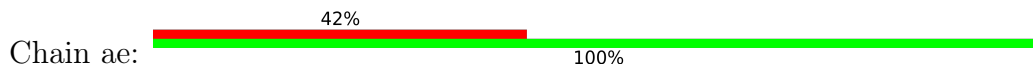


• Molecule 1: Major capsid protein (MCP)

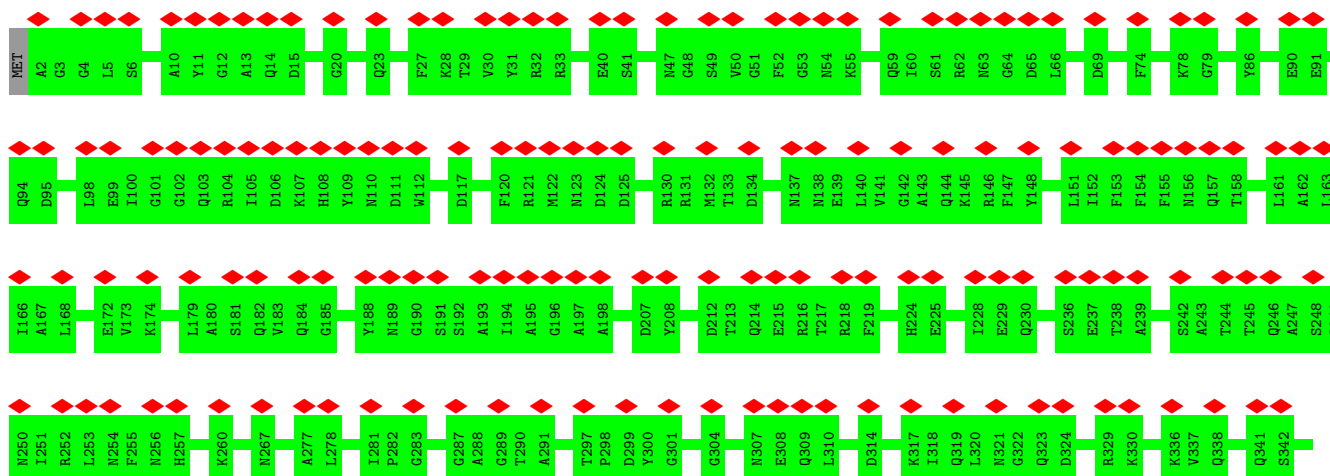


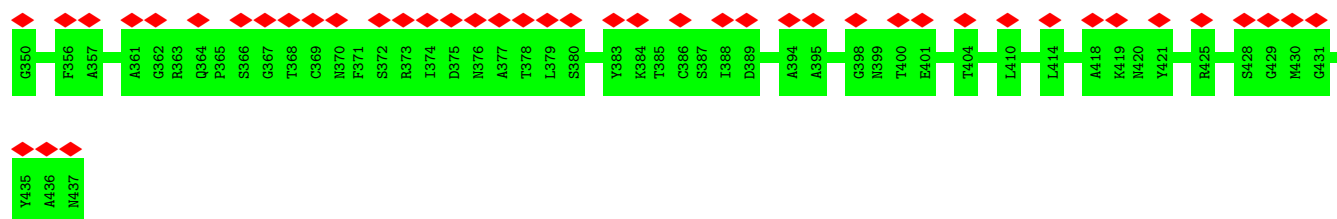


• Molecule 1: Major capsid protein (MCP)



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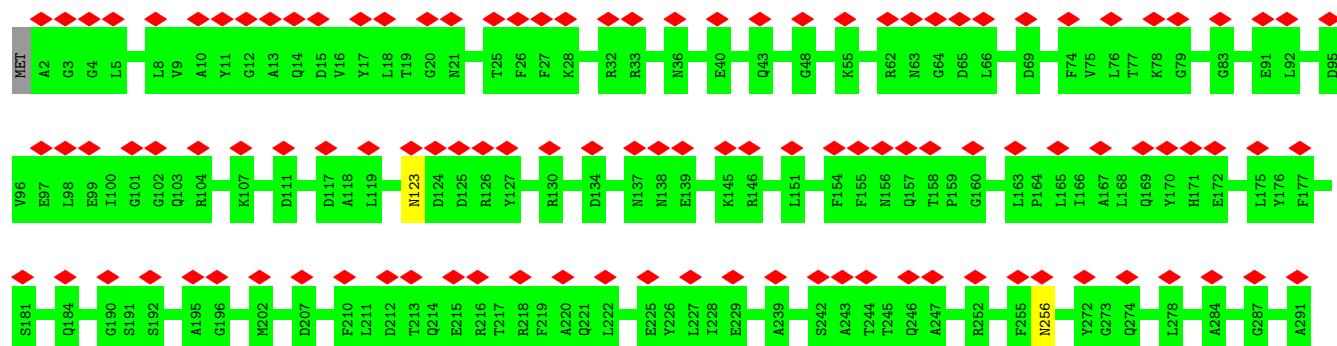
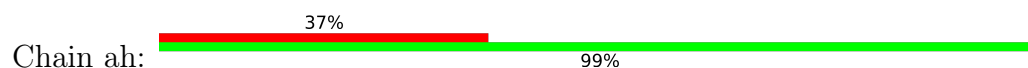


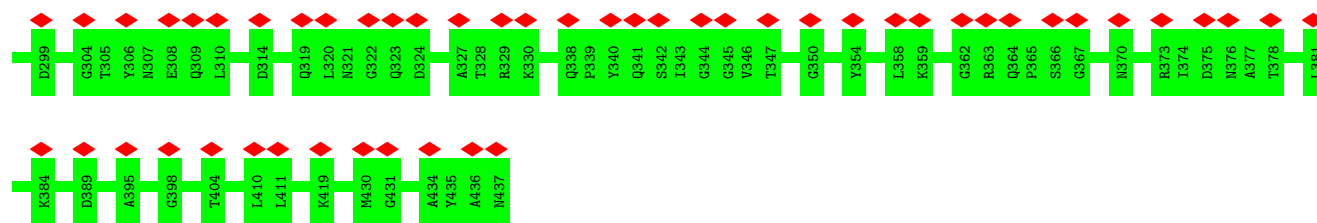


• Molecule 1: Major capsid protein (MCP)



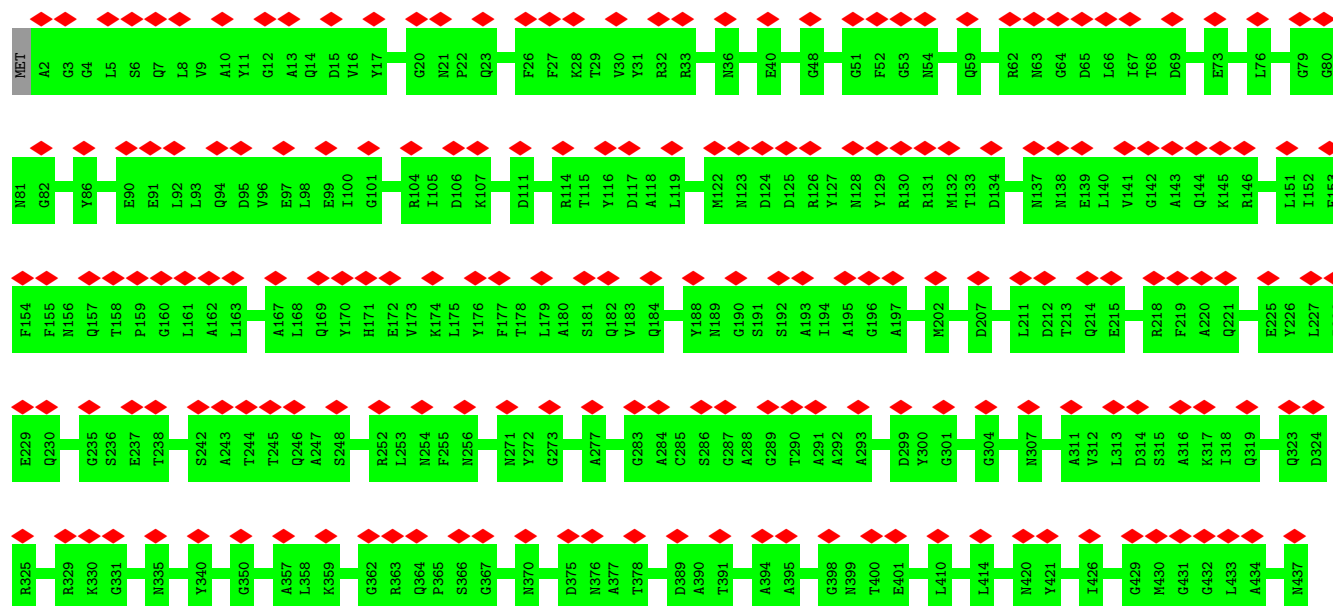
• Molecule 1: Major capsid protein (MCP)





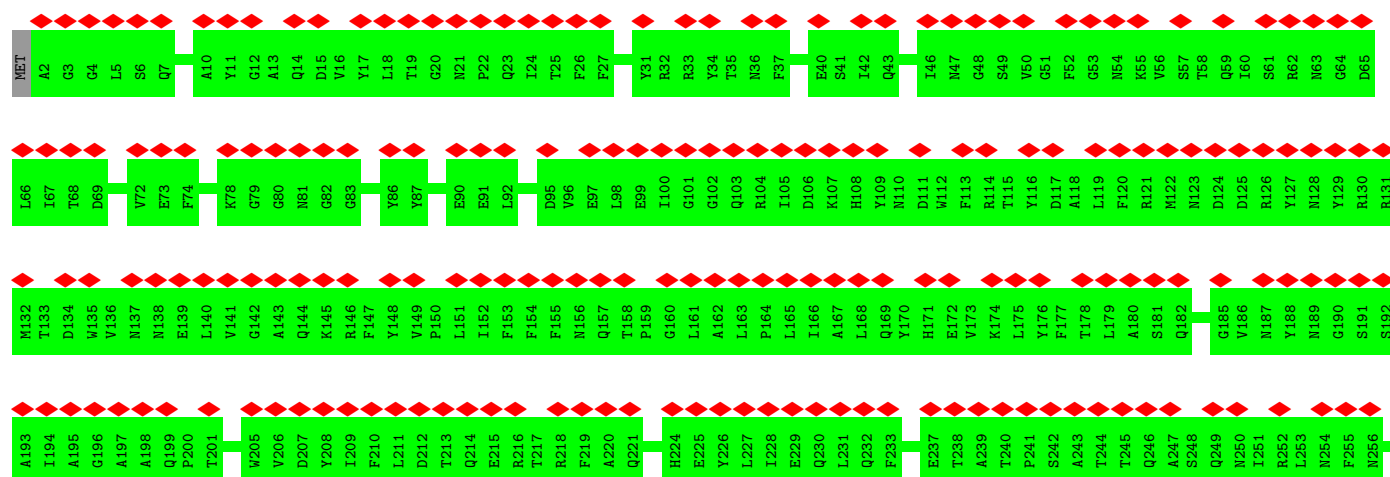
• Molecule 1: Major capsid protein (MCP)

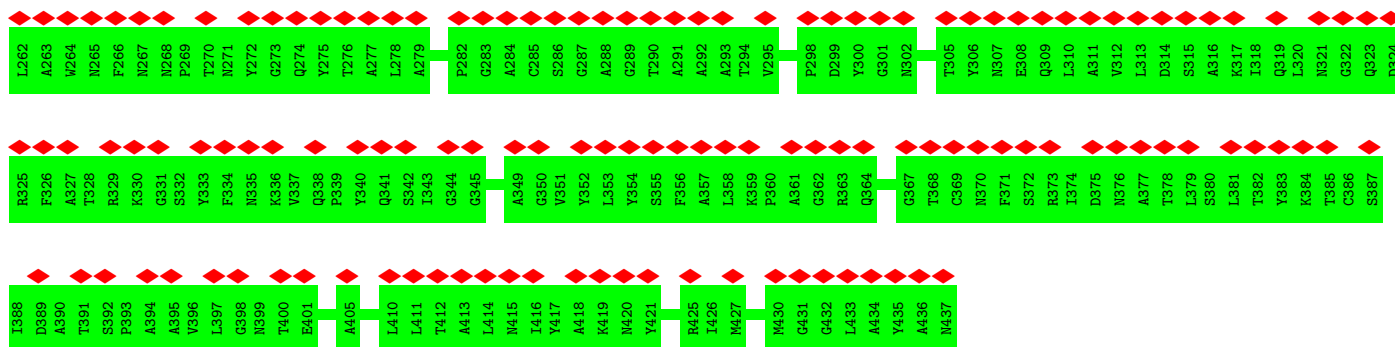
Chain ai: 44%
100%



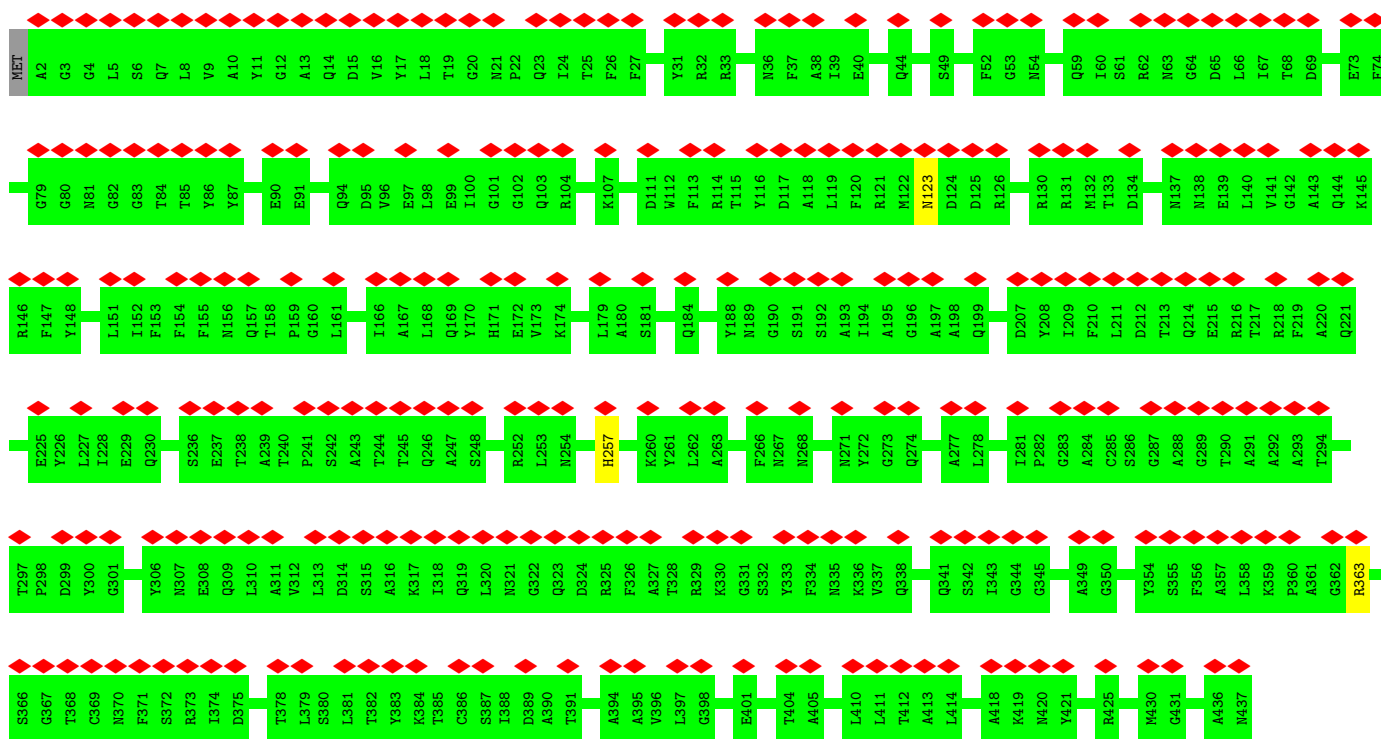
• Molecule 1: Major capsid protein (MCP)

Chain aj: 75%
100%

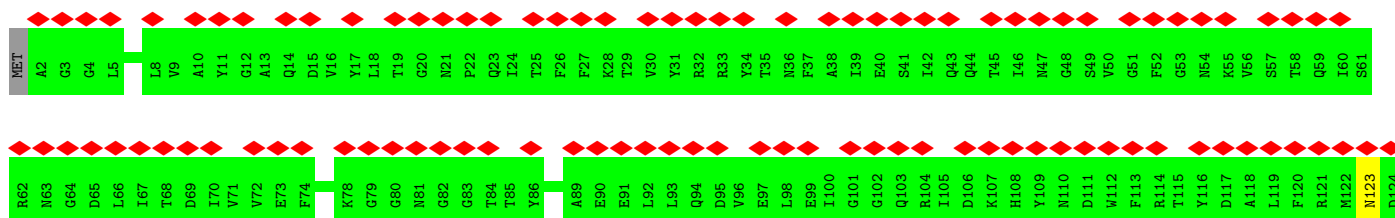
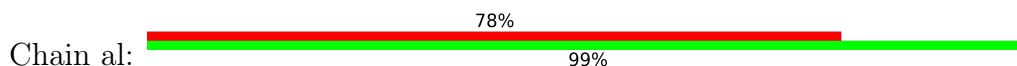


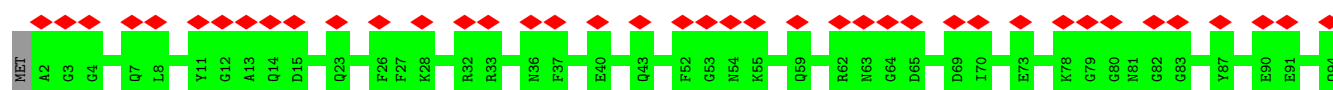


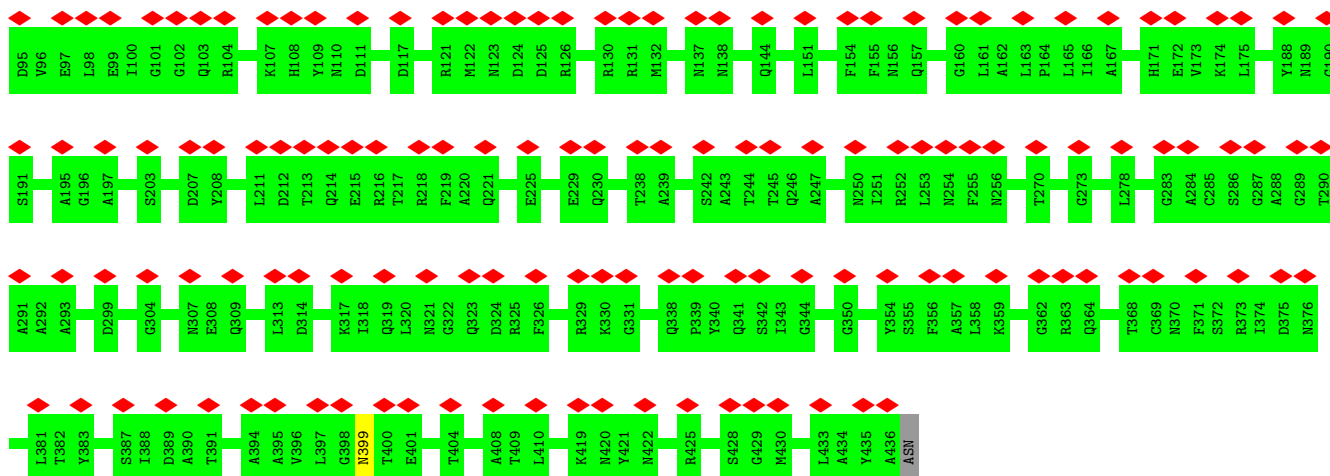
• Molecule 1: Major capsid protein (MCP)



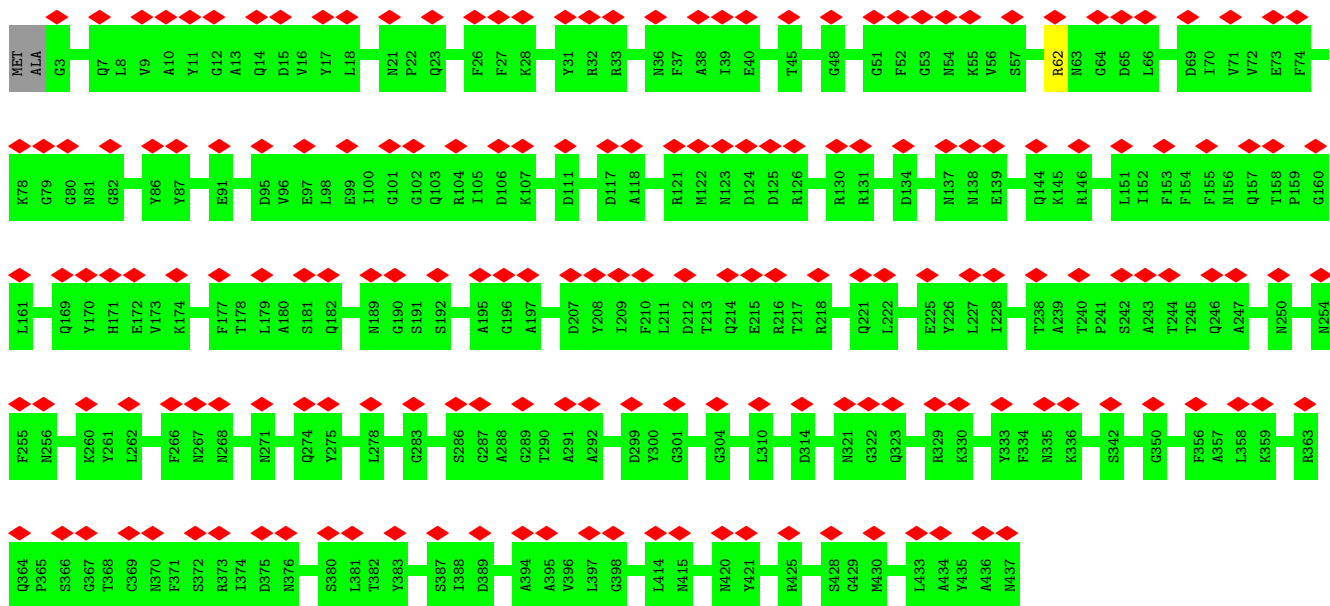
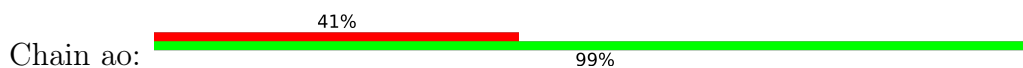
• Molecule 1: Major capsid protein (MCP)



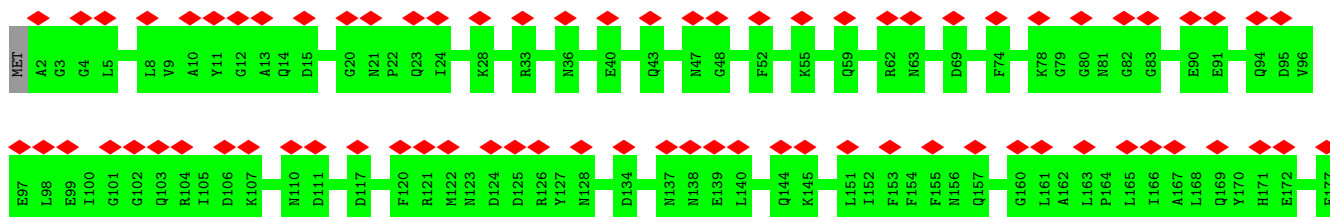
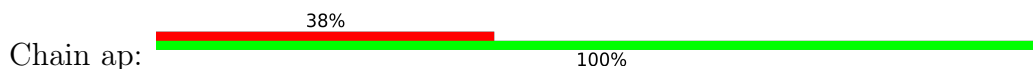


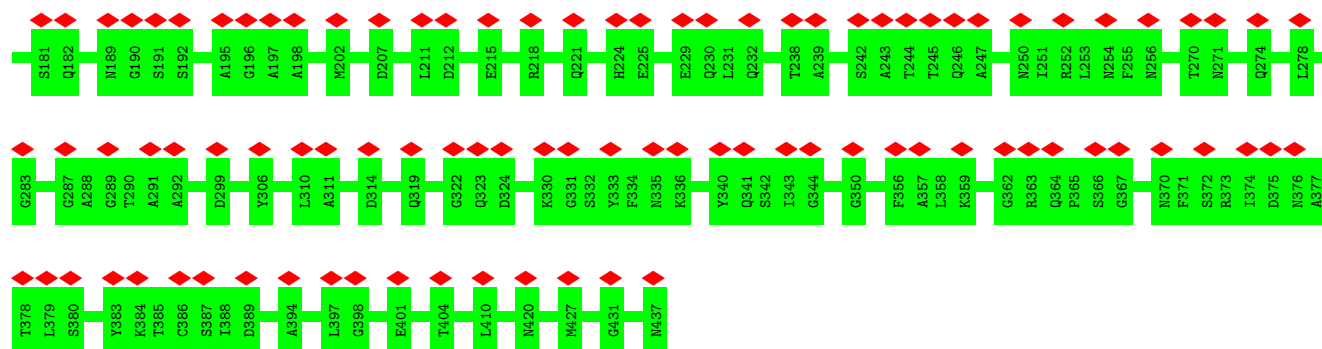


• Molecule 1: Major capsid protein (MCP)

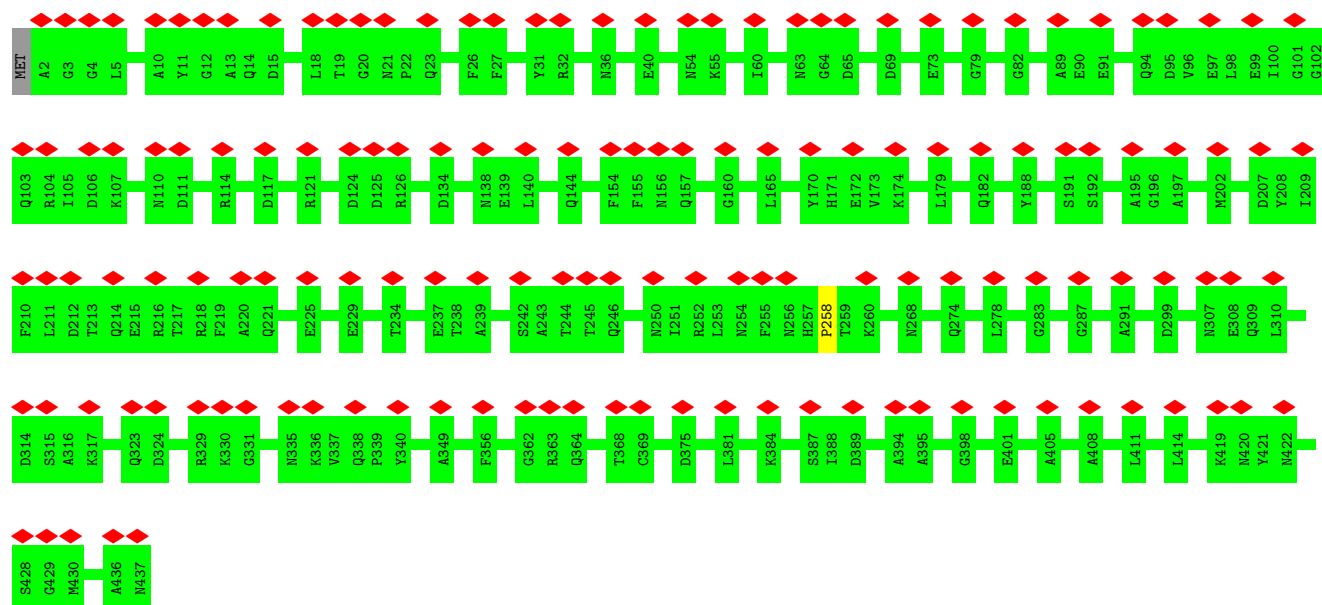


• Molecule 1: Major capsid protein (MCP)

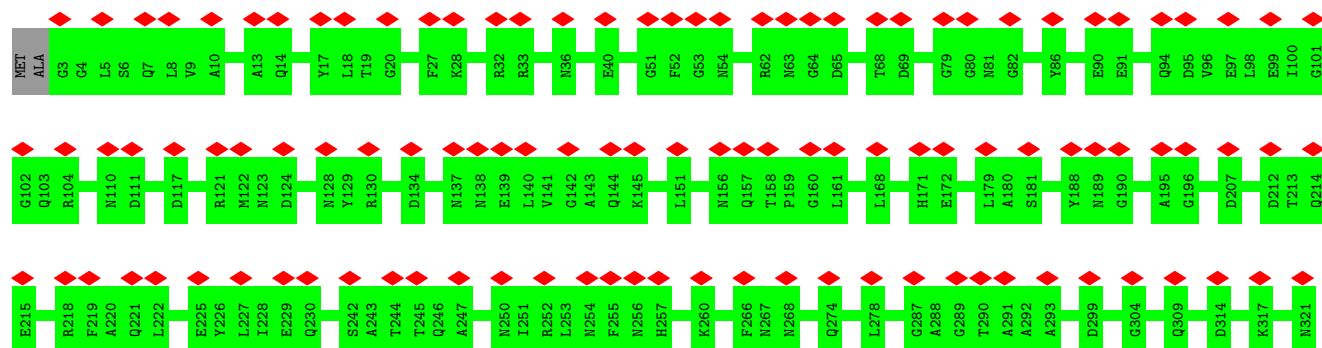


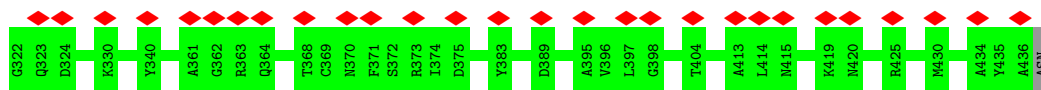


• Molecule 1: Major capsid protein (MCP)



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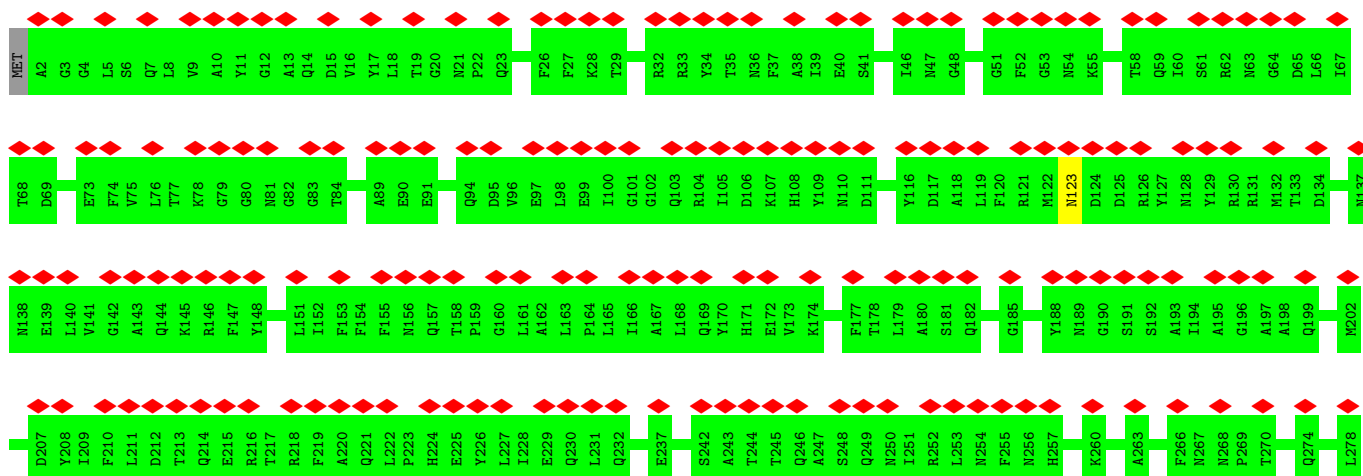
• Molecule 1: Major capsid protein (MCP)

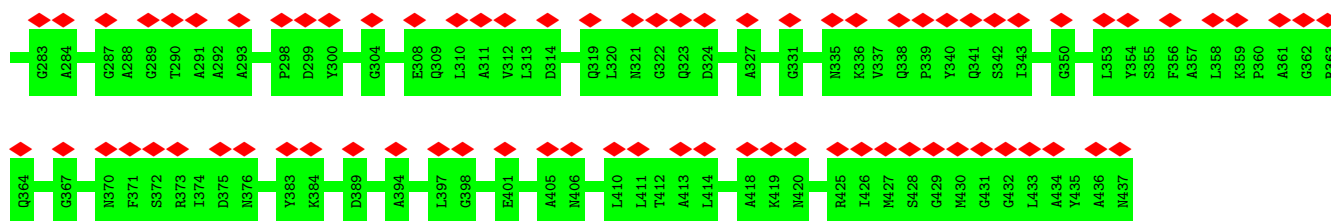
Chain as: 44% 99%



• Molecule 1: Major capsid protein (MCP)

Chain at: 58% 100%

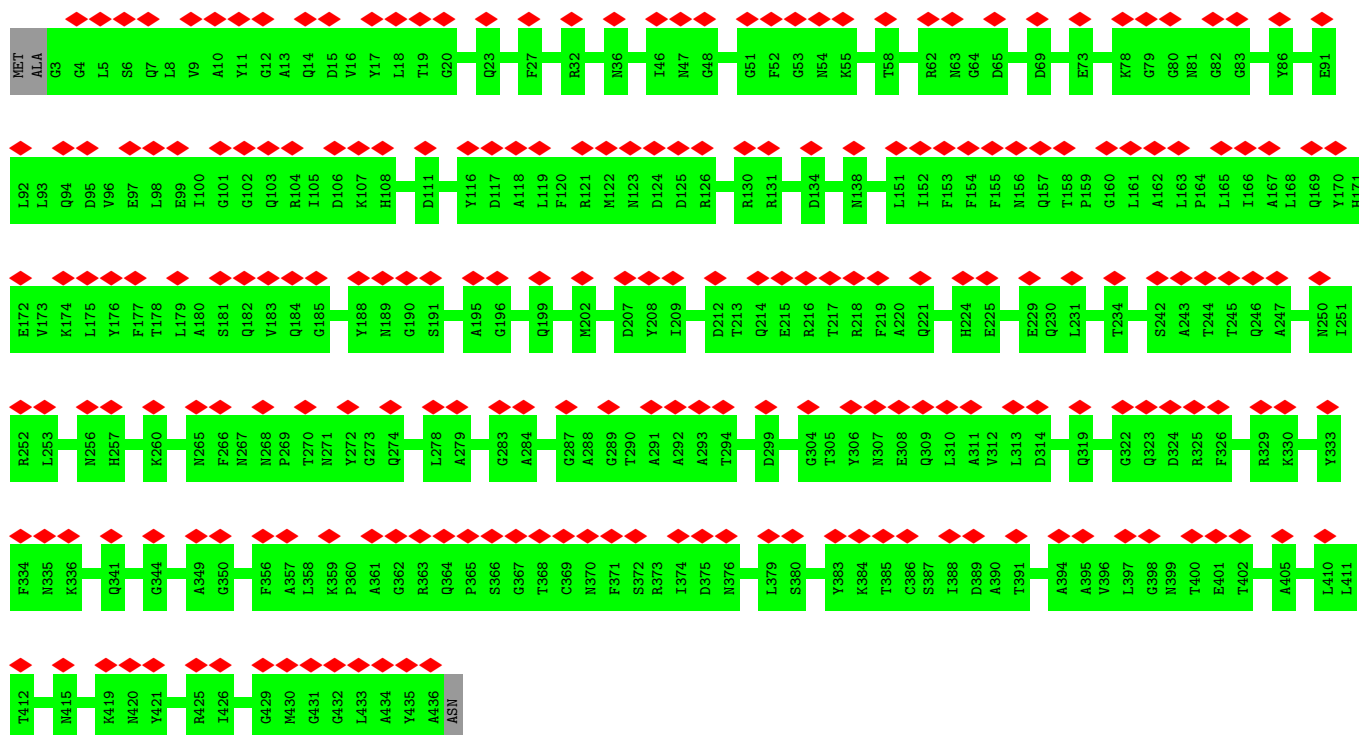




• Molecule 1: Major capsid protein (MCP)



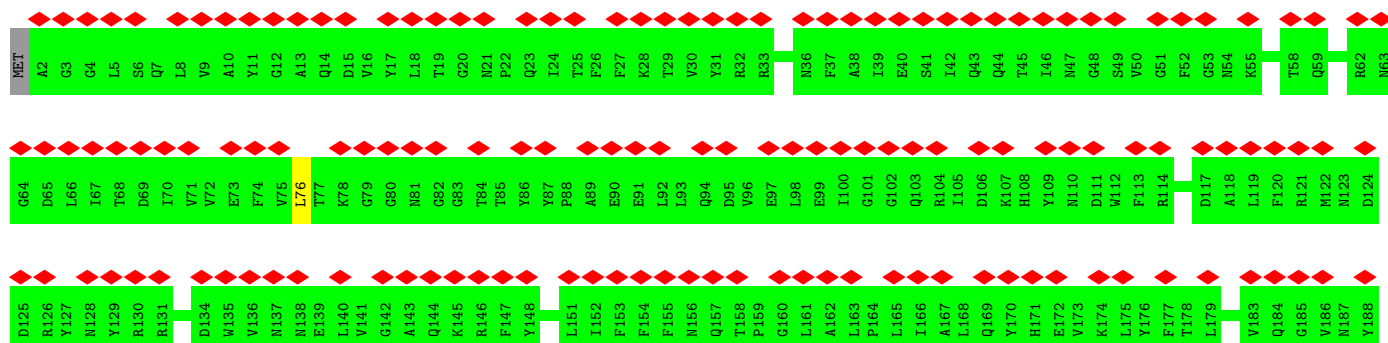
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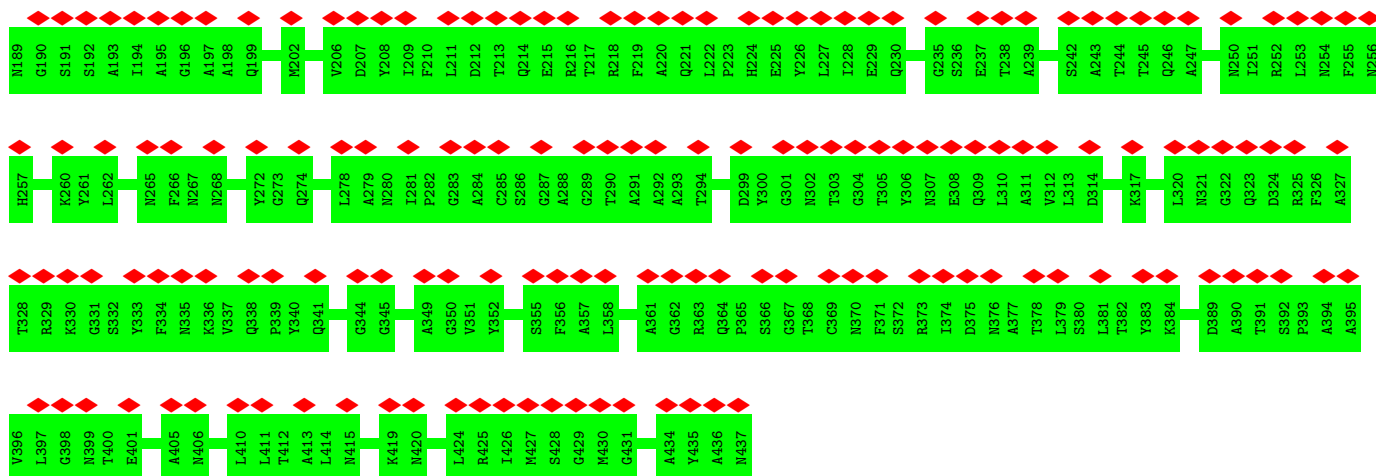


• Molecule 1: Major capsid protein (MCP)

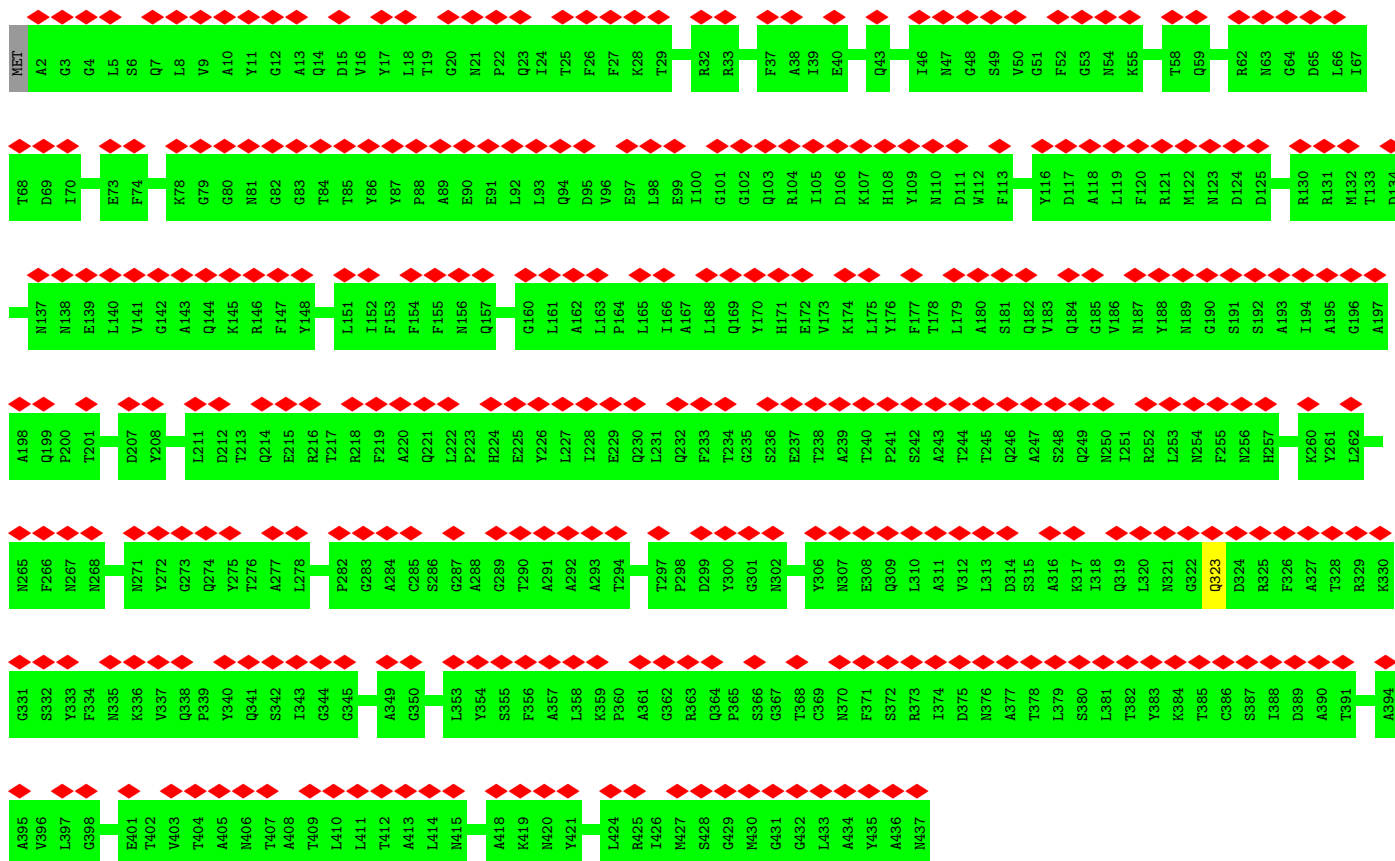
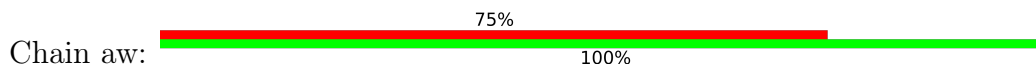


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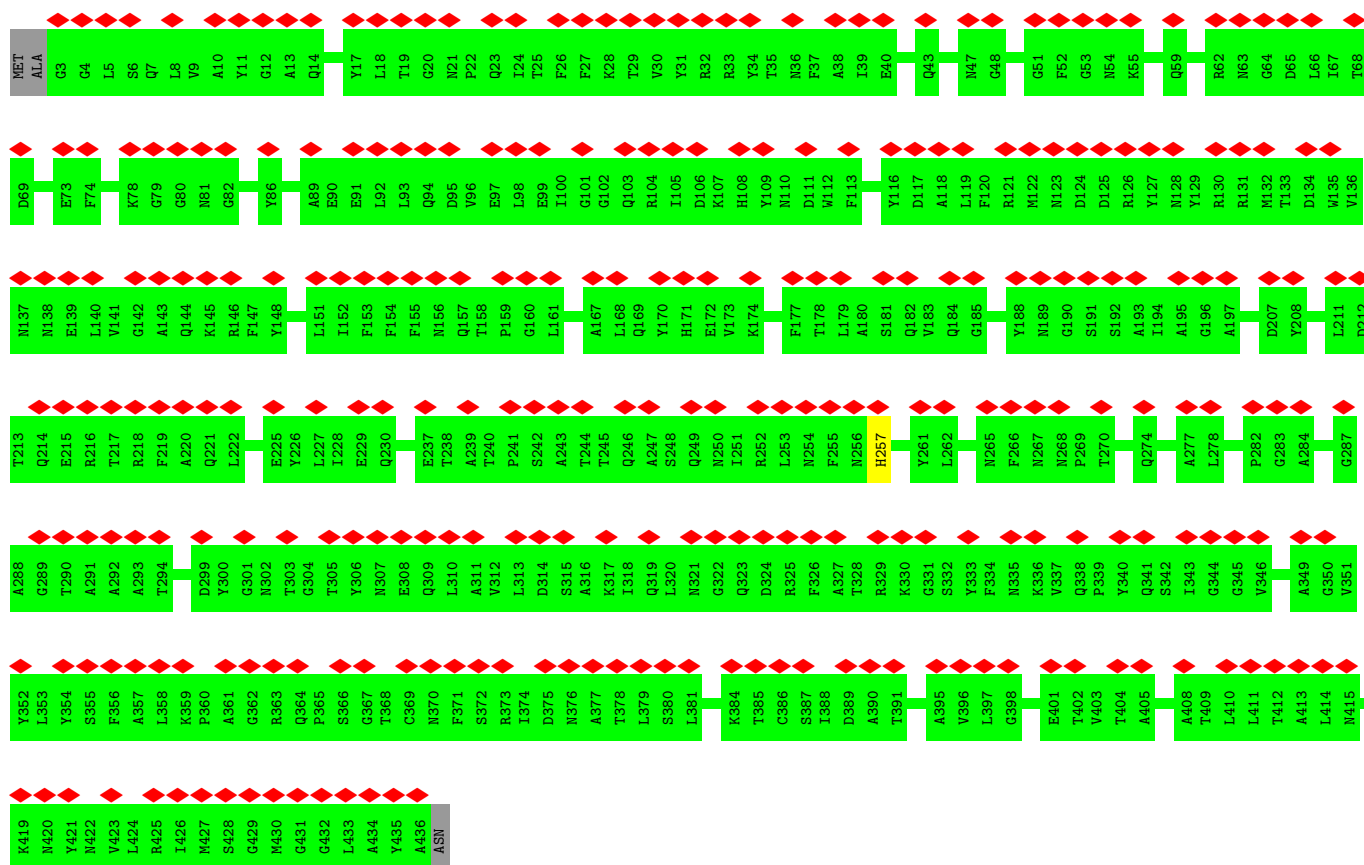


• Molecule 1: Major capsid protein (MCP)

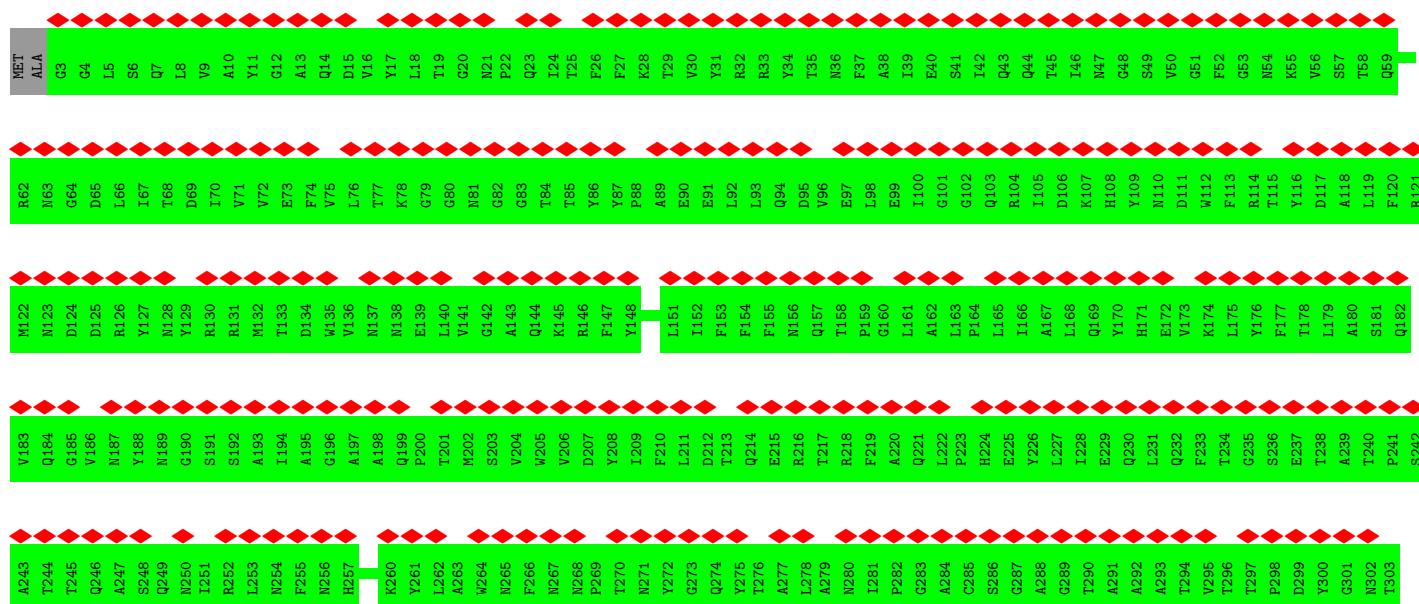
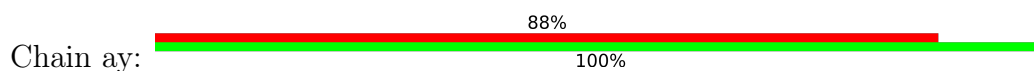


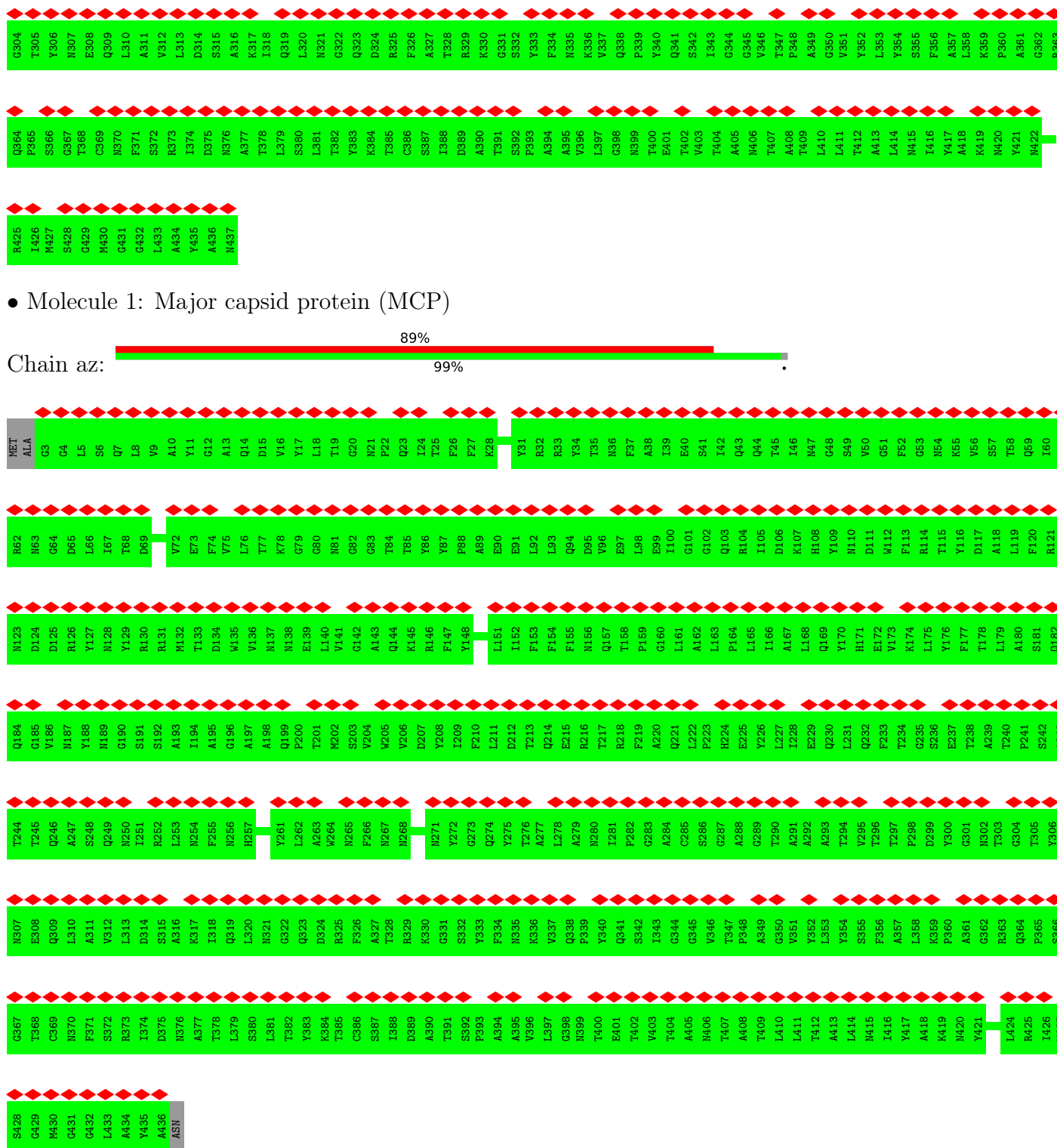
• Molecule 1: Major capsid protein (MCP)



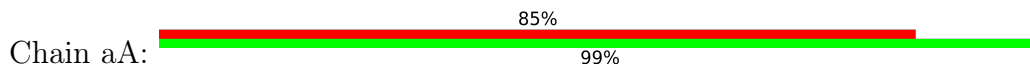


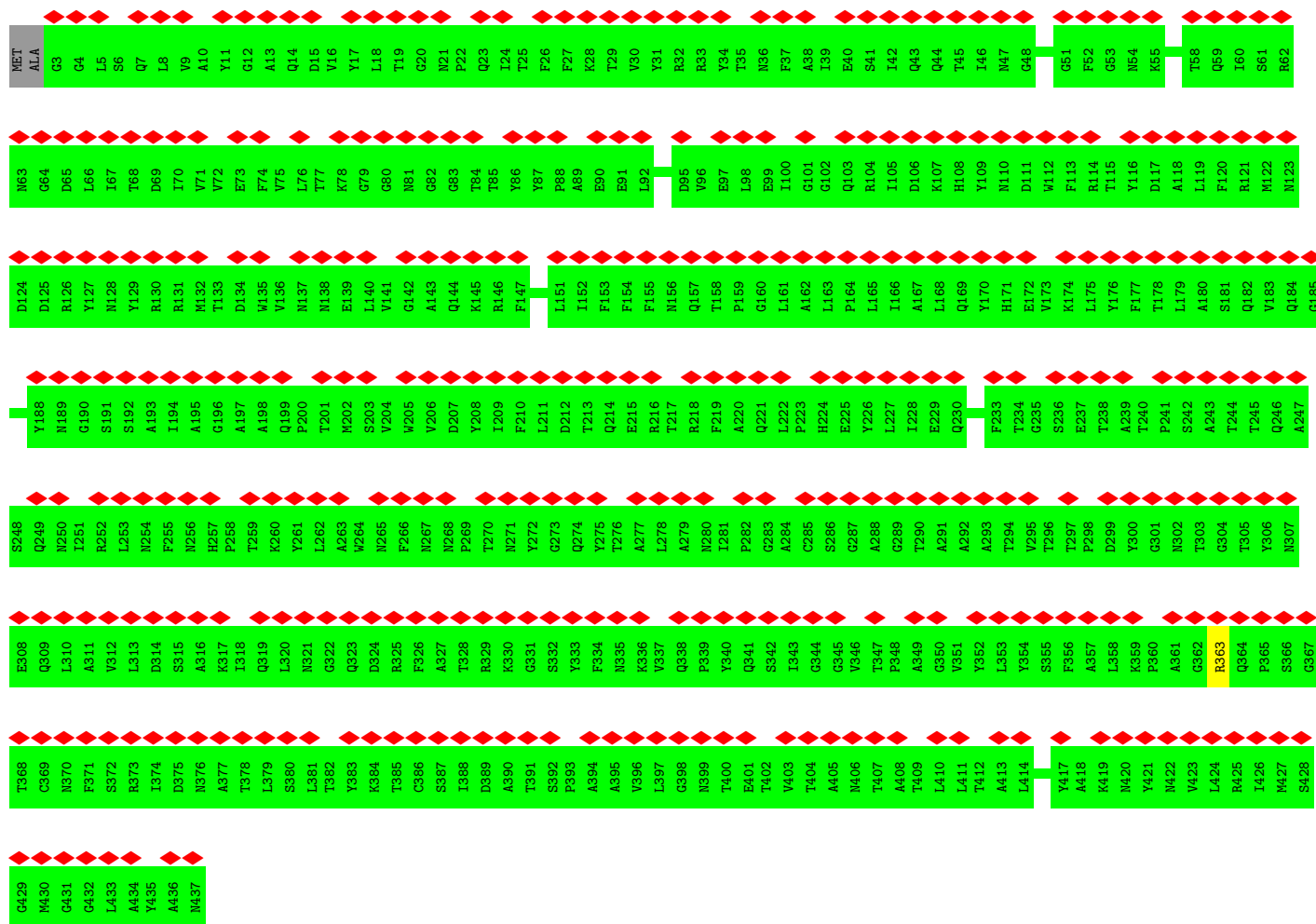
• Molecule 1: Major capsid protein (MCP)



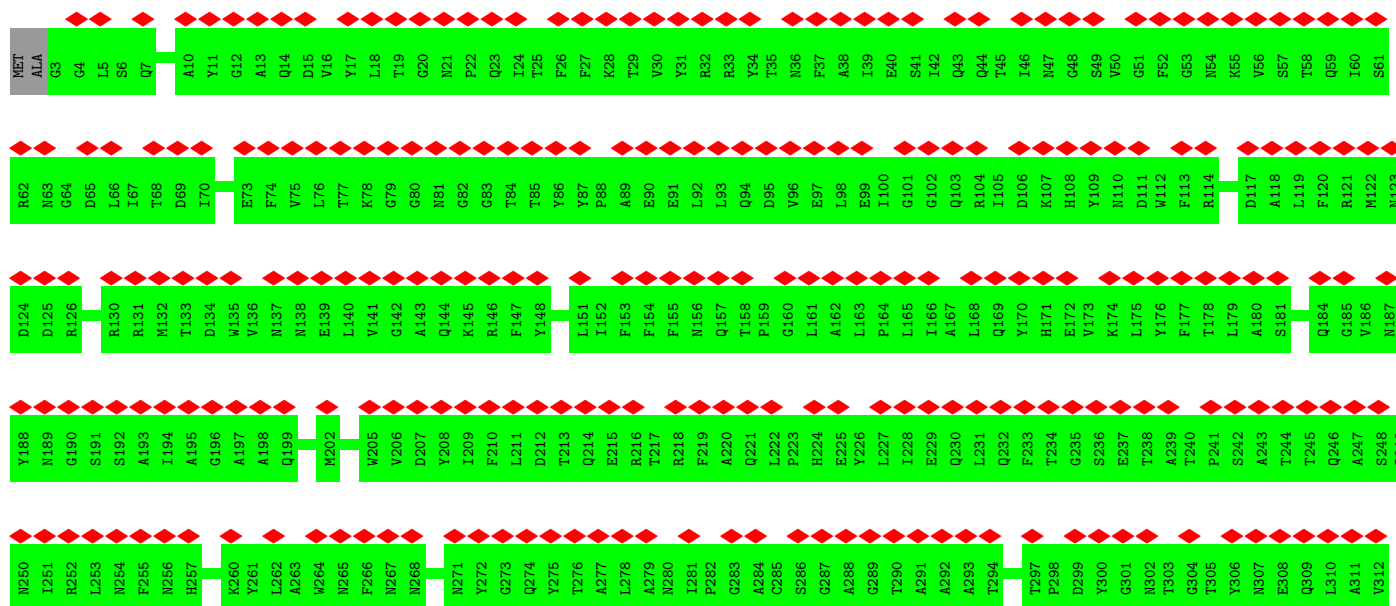
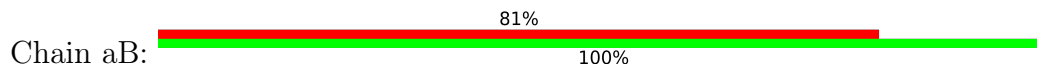


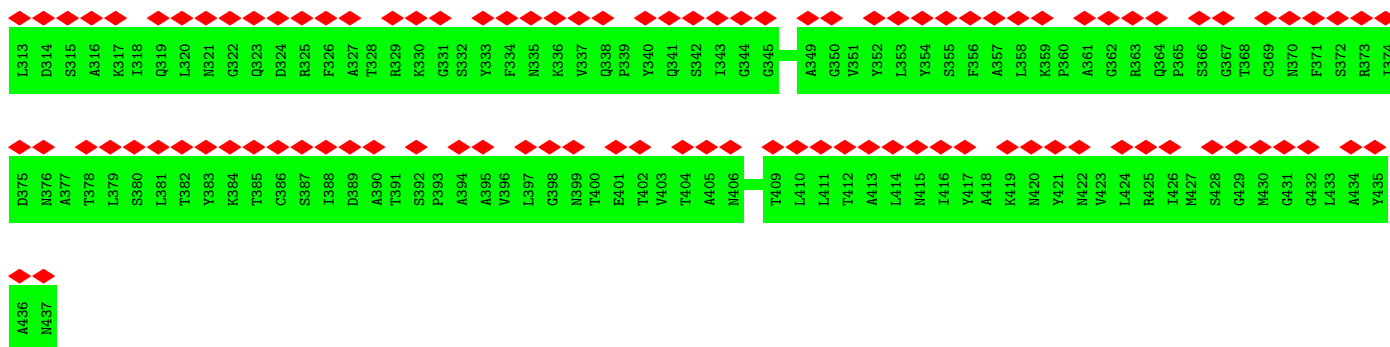
- Molecule 1: Major capsid protein (MCP)



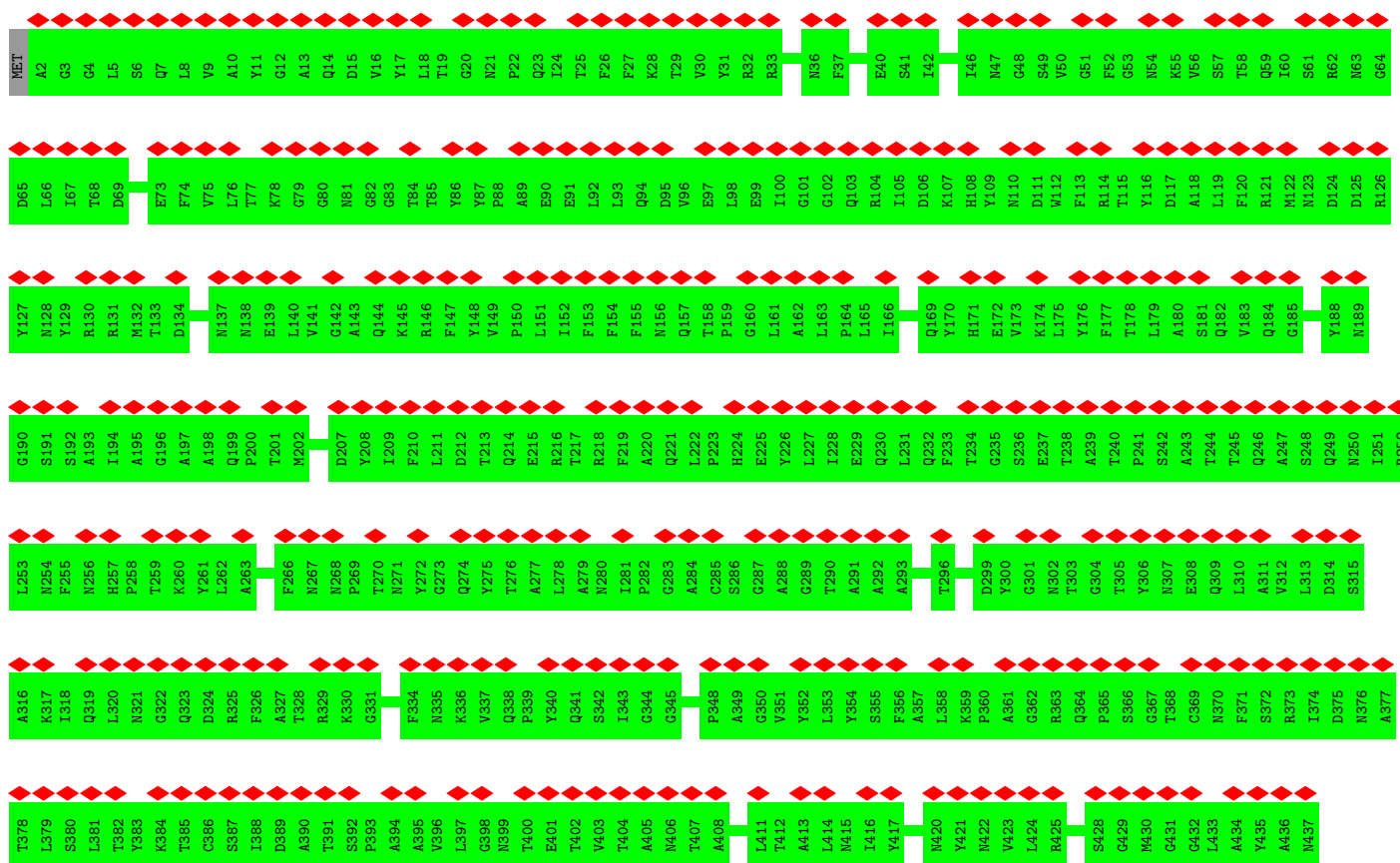
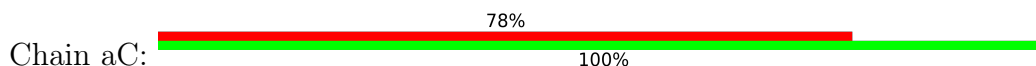


• Molecule 1: Major capsid protein (MCP)

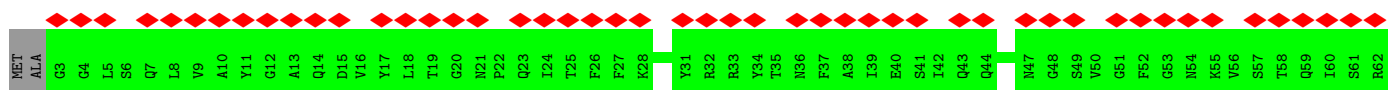
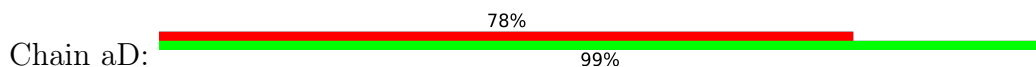


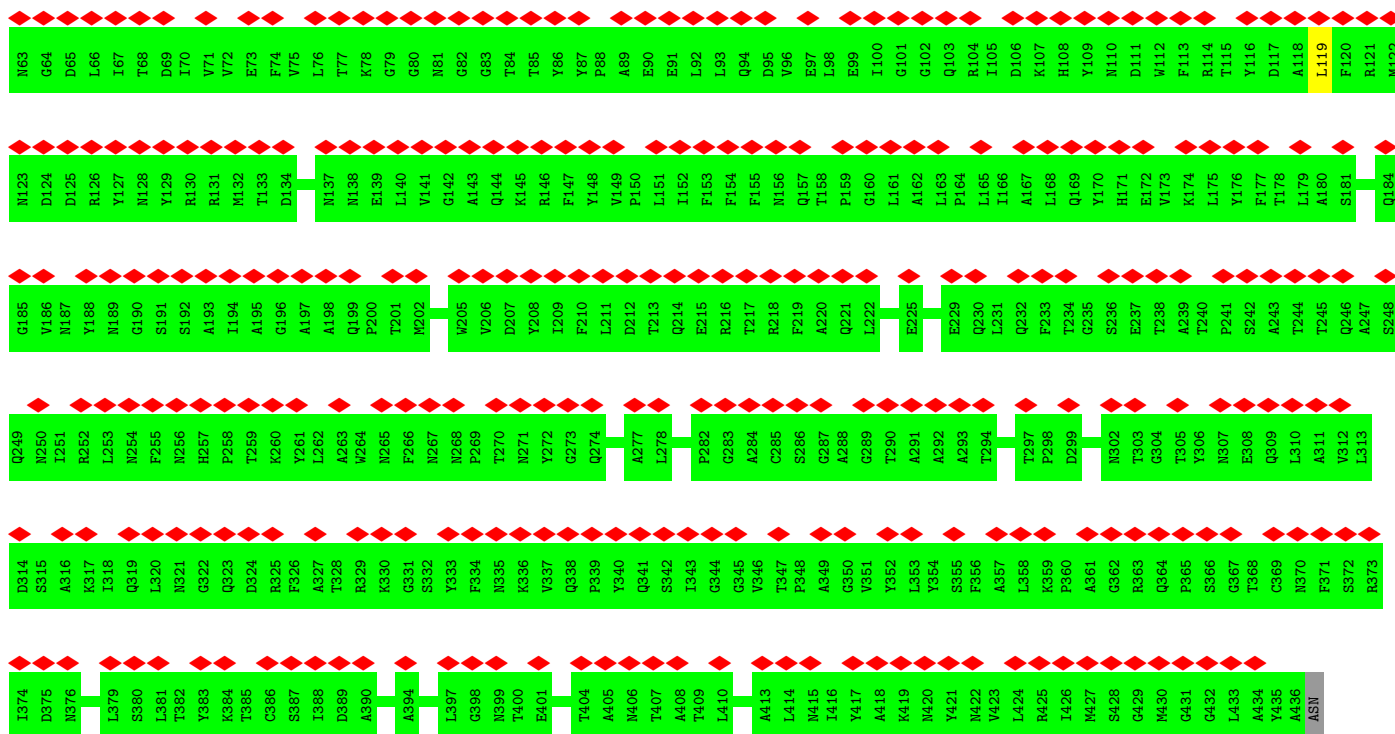


• Molecule 1: Major capsid protein (MCP)



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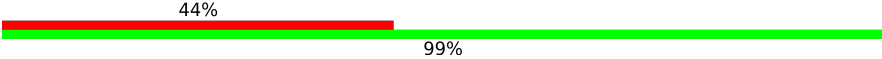


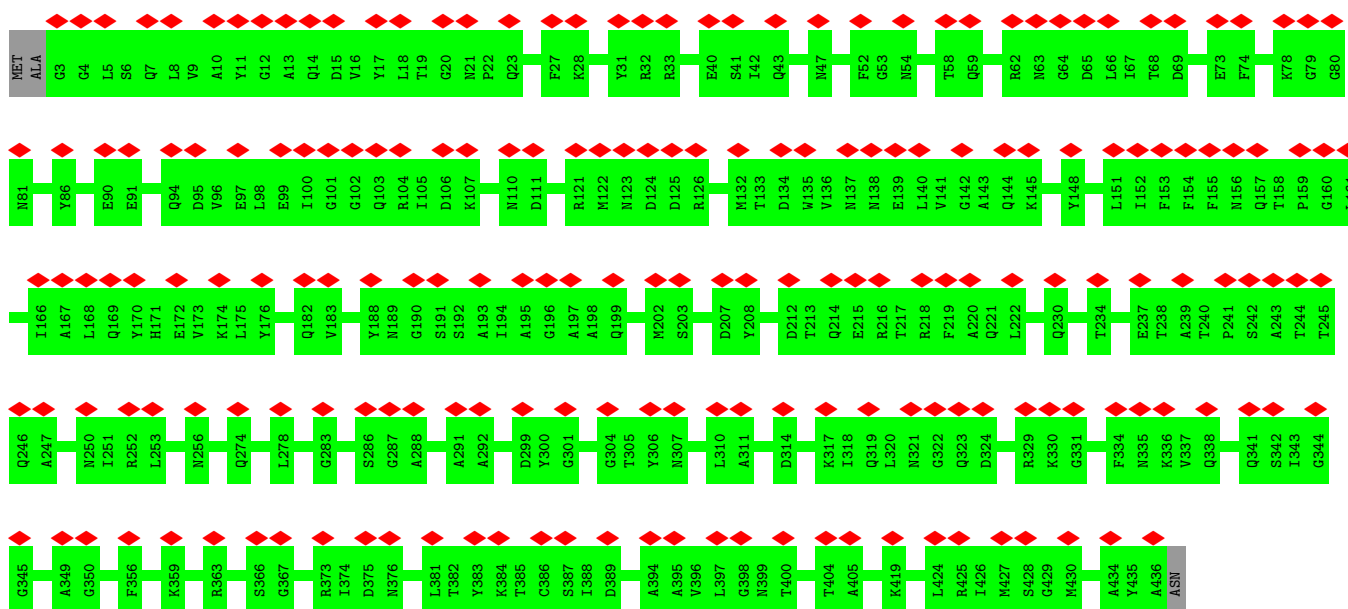


• Molecule 1: Major capsid protein (MCP)



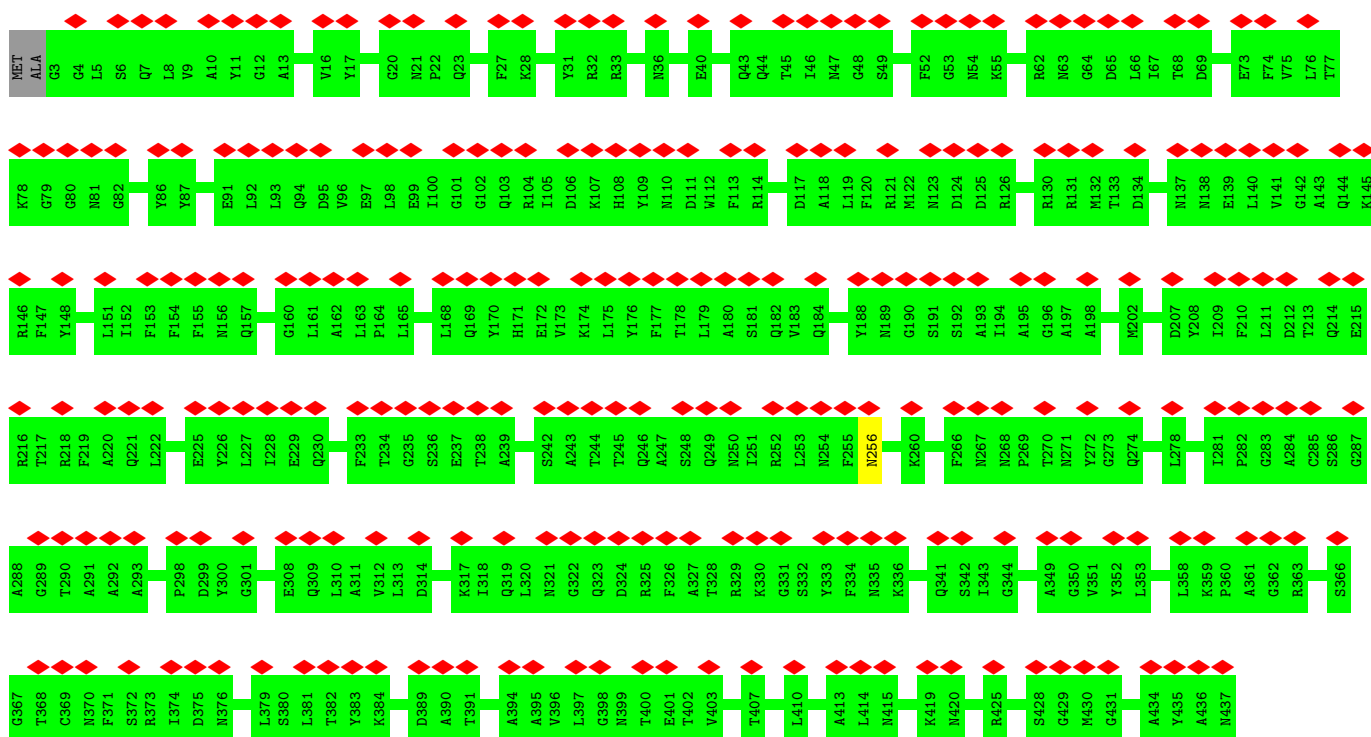
• Molecule 1: Major capsid protein (MCP)

Chain aF: 

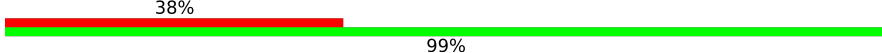


• Molecule 1: Major capsid protein (MCP)

Chain aG: 

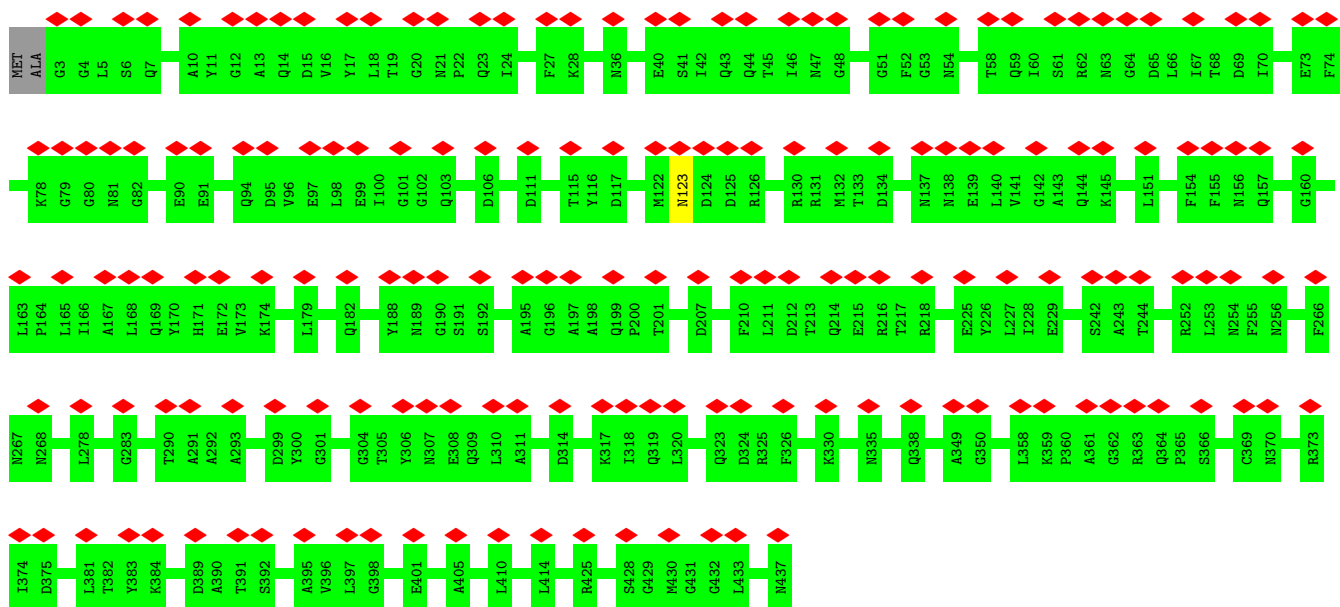


• Molecule 1: Major capsid protein (MCP)

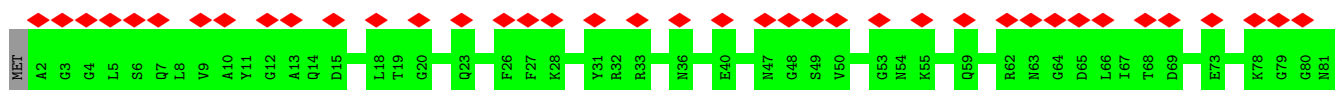
Chain aH: 

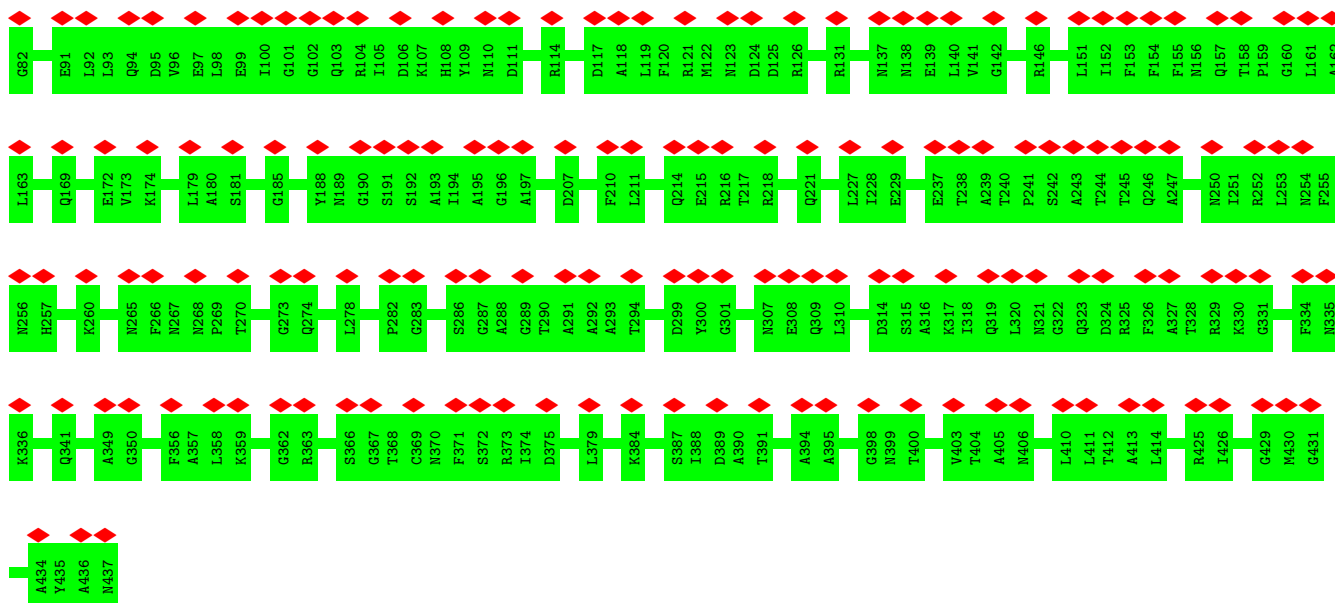


• Molecule 1: Major capsid protein (MCP)



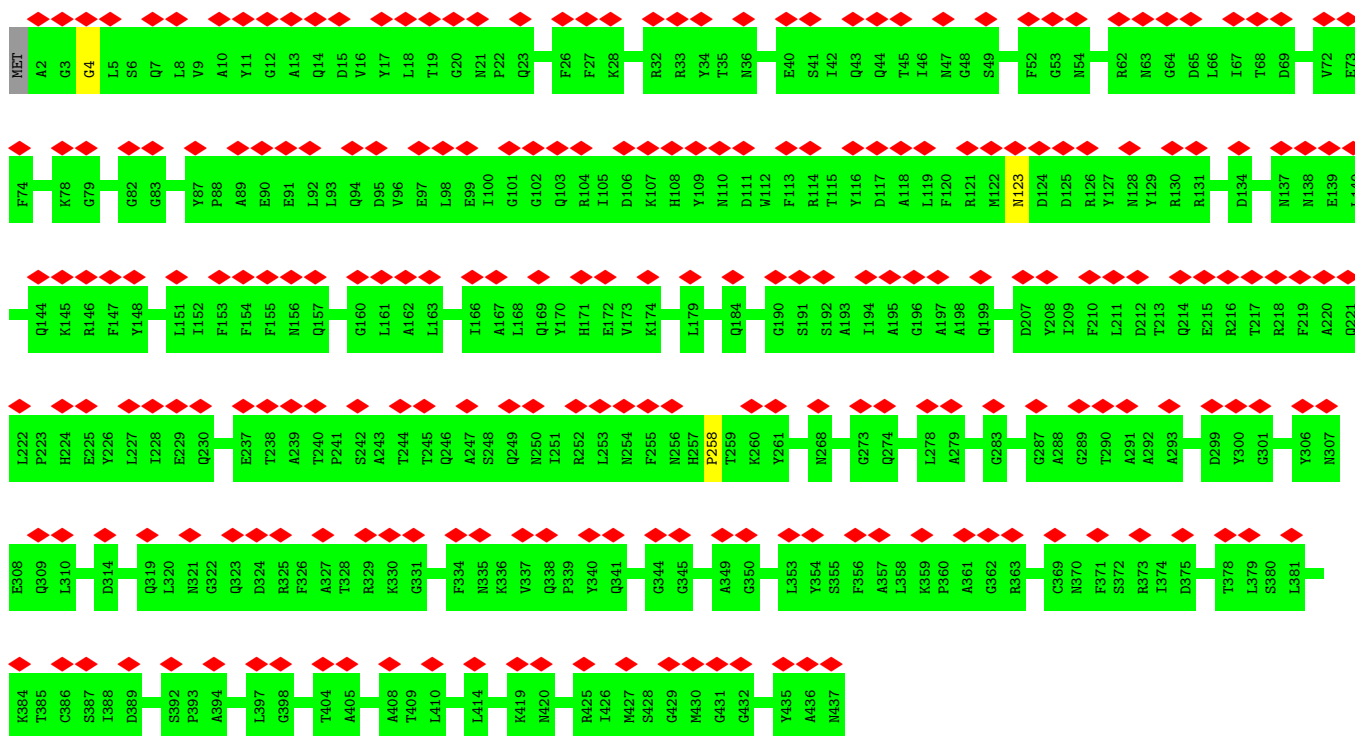
• Molecule 1: Major capsid protein (MCP)





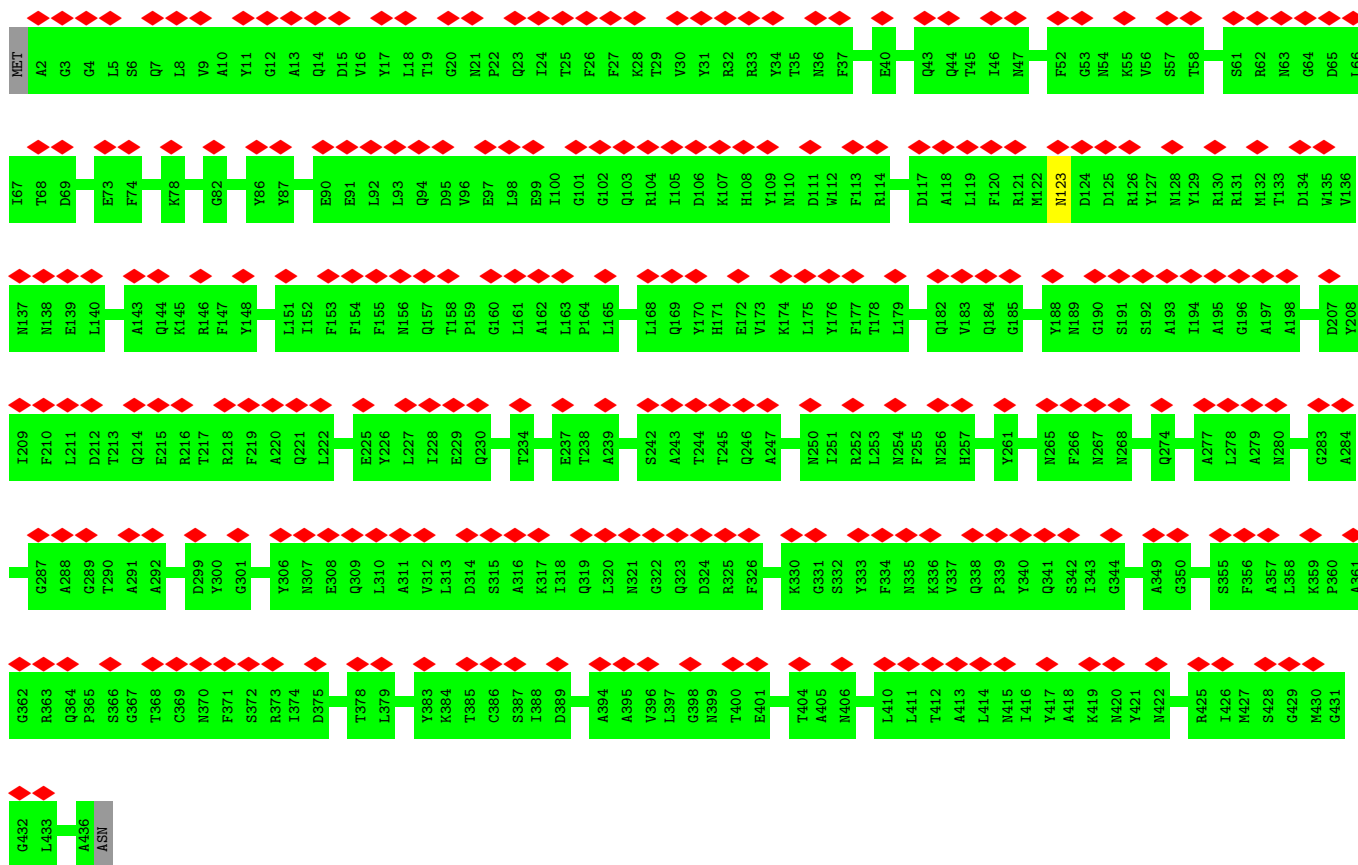
• Molecule 1: Major capsid protein (MCP)

Chain aK: 54% 99%

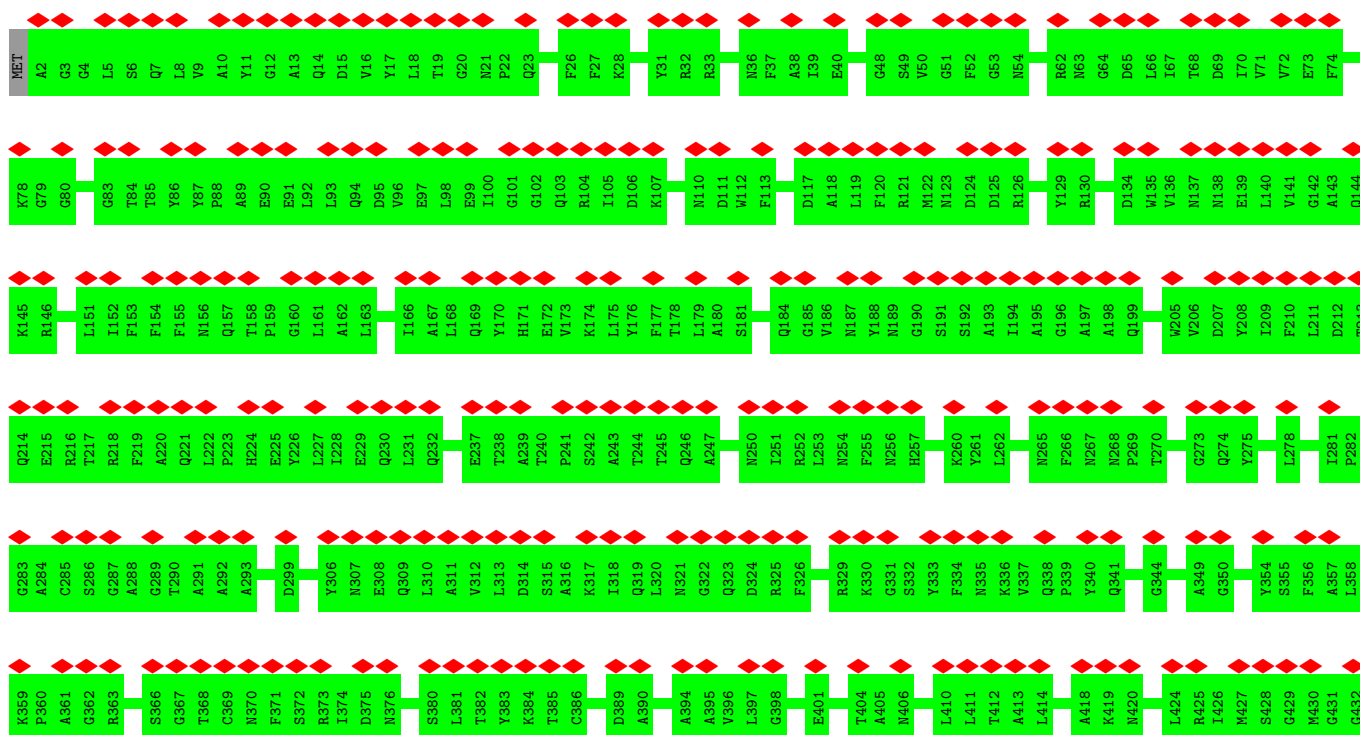


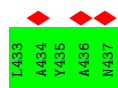
• Molecule 1: Major capsid protein (MCP)

Chain aL: 60% 99%

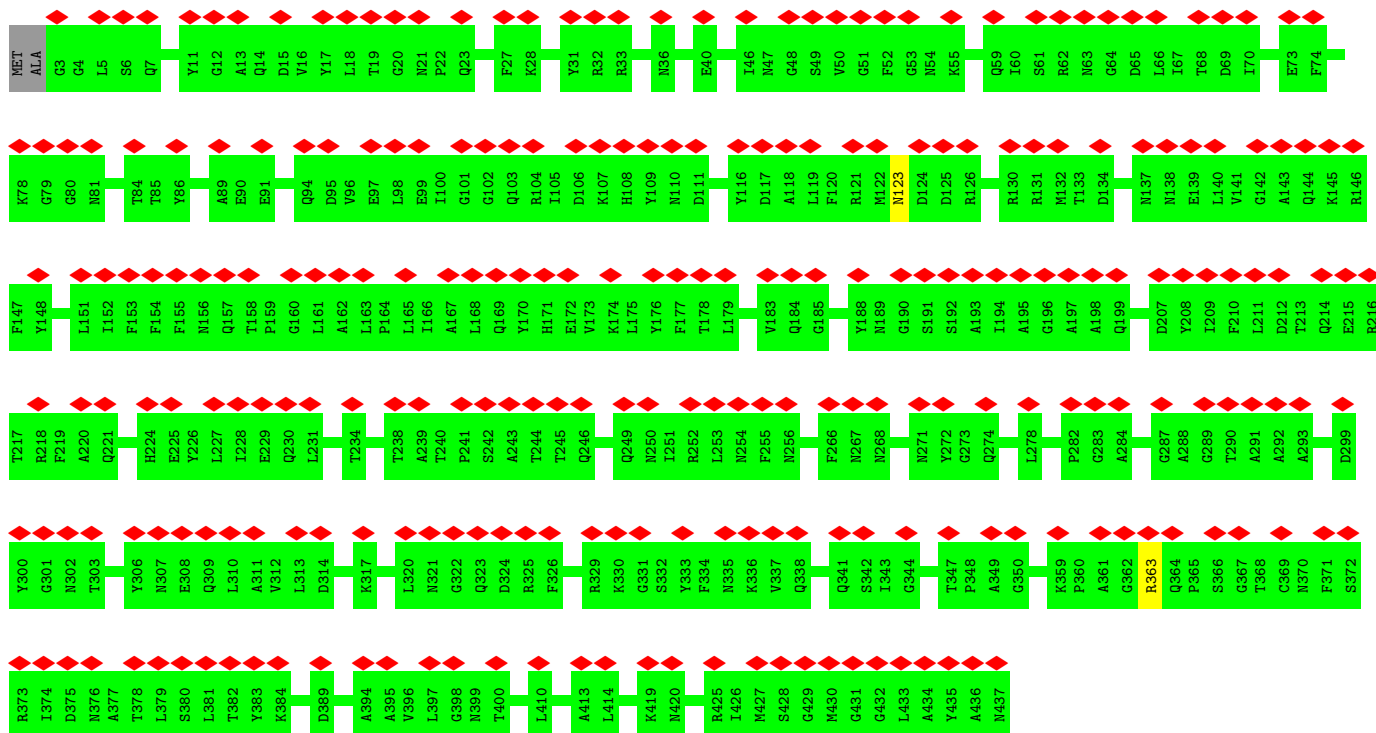


• Molecule 1: Major capsid protein (MCP)

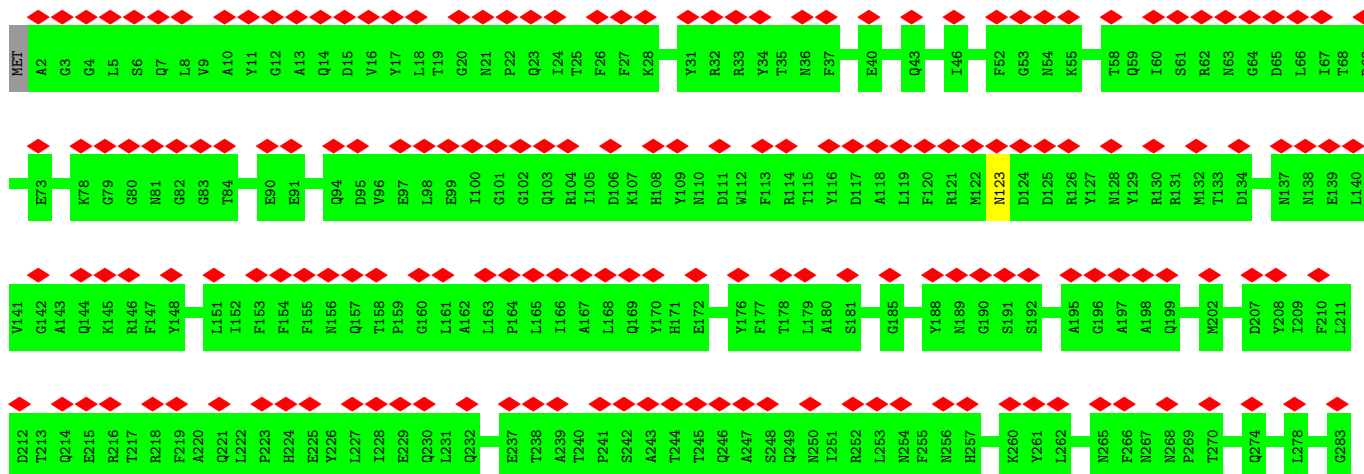


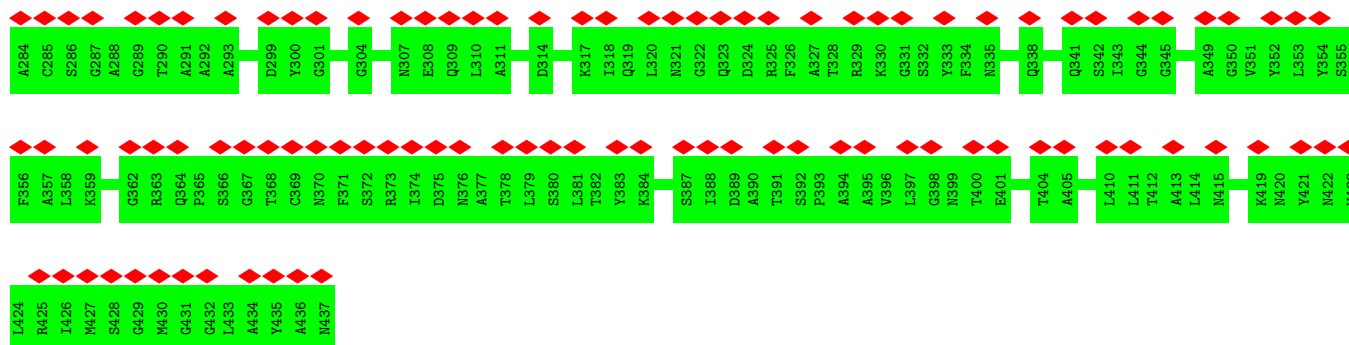


• Molecule 1: Major capsid protein (MCP)



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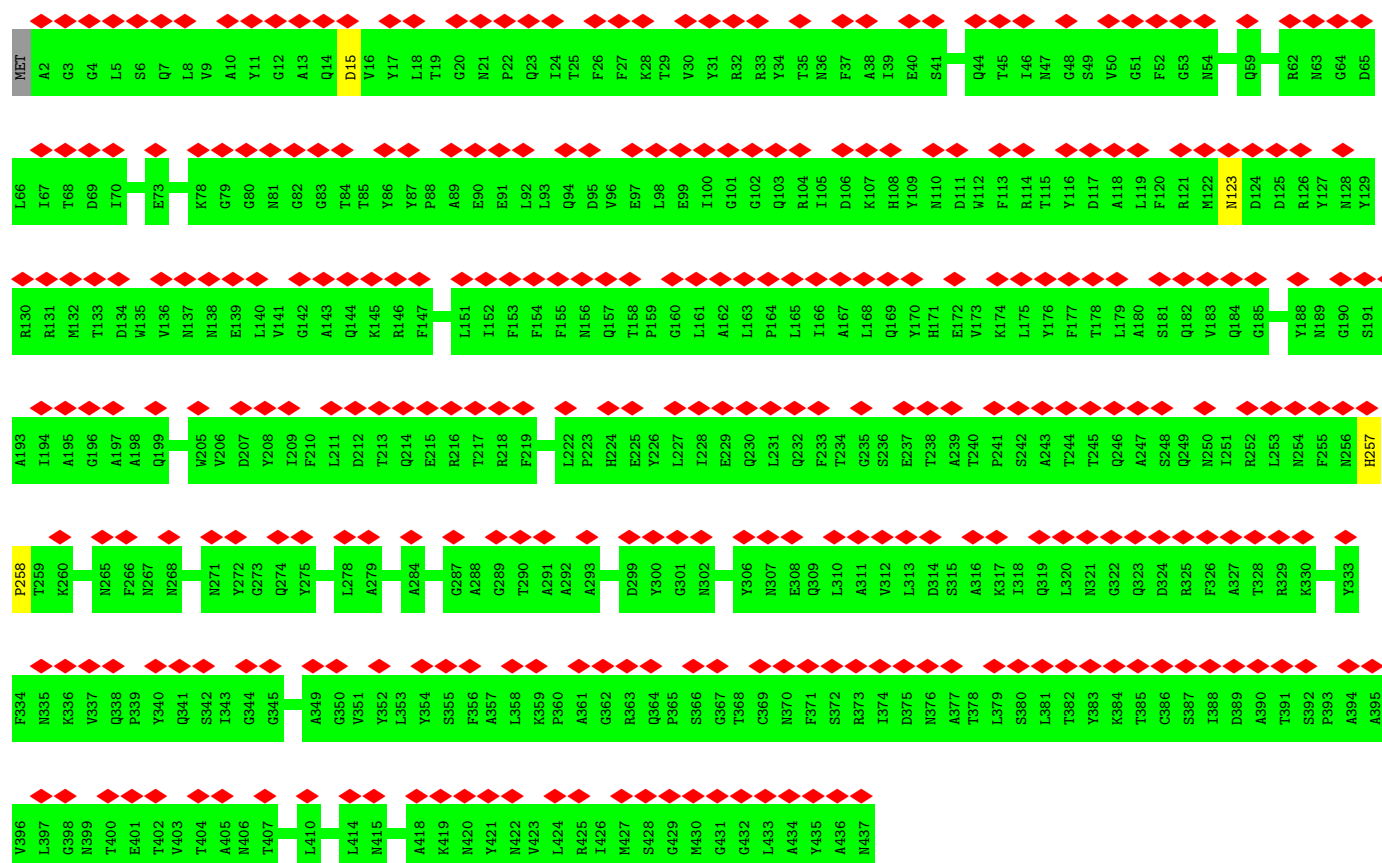
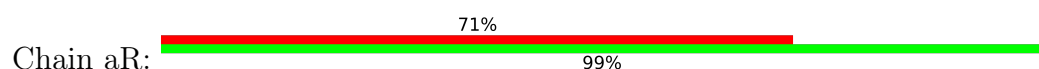


• Molecule 1: Major capsid protein (MCP)

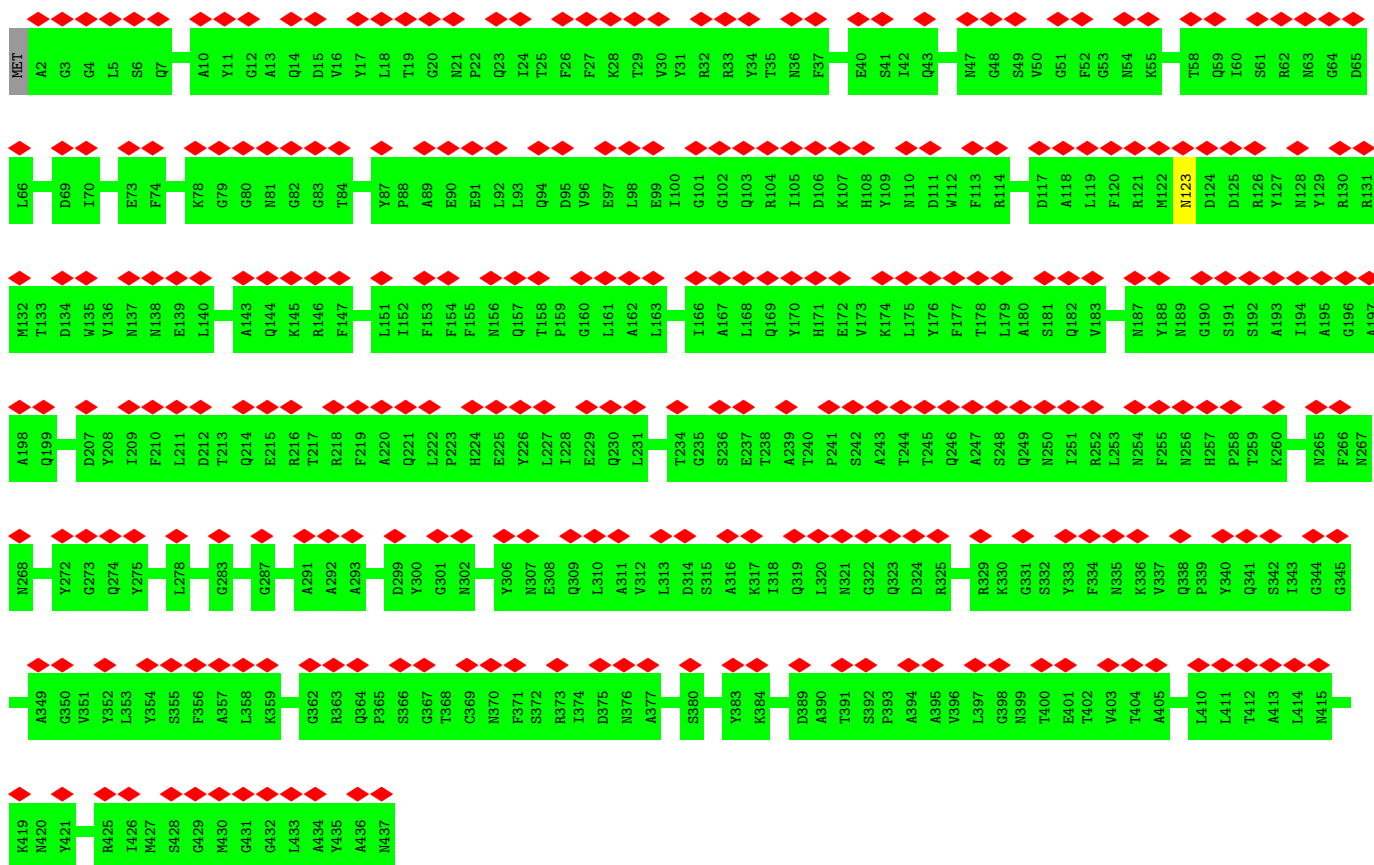




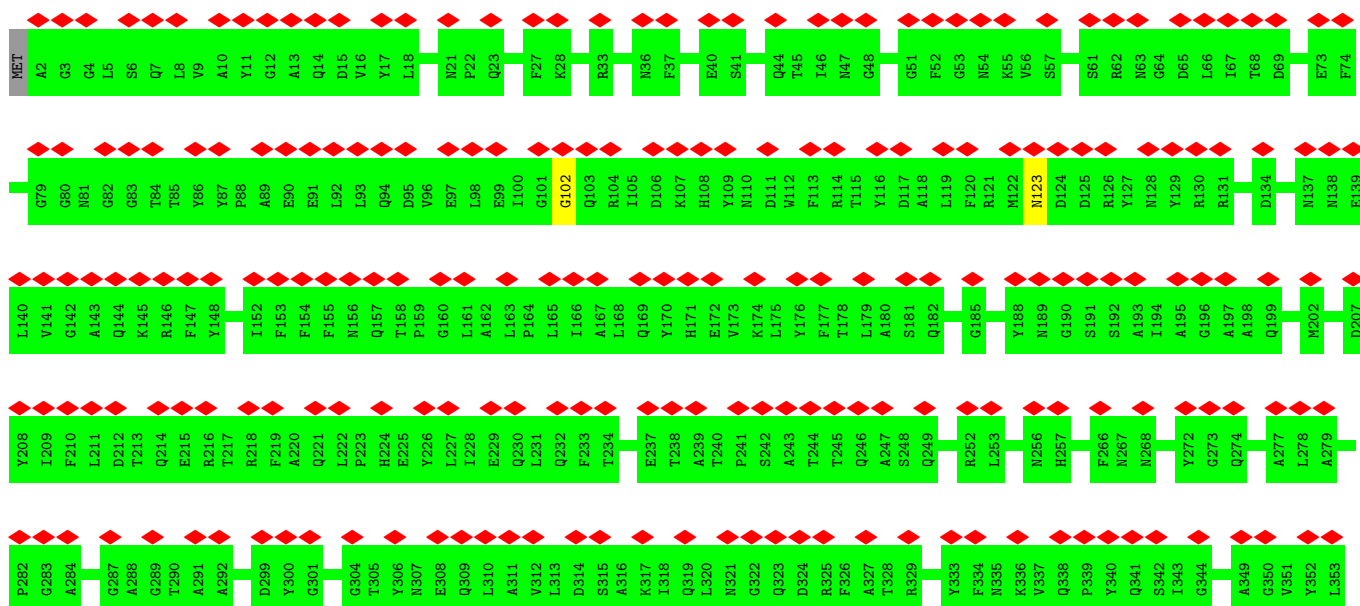
• Molecule 1: Major capsid protein (MCP)

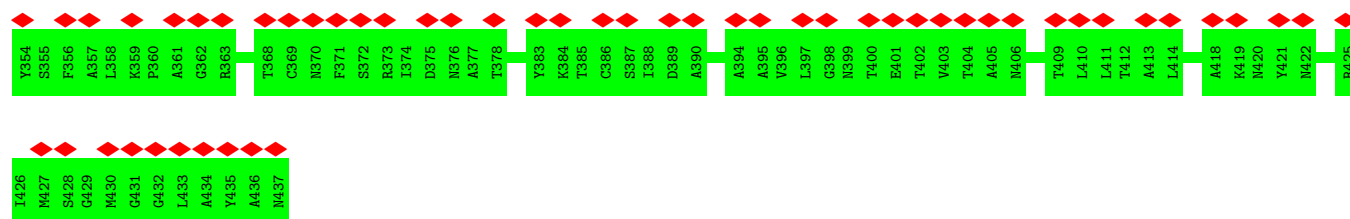


• Molecule 1: Major capsid protein (MCP)

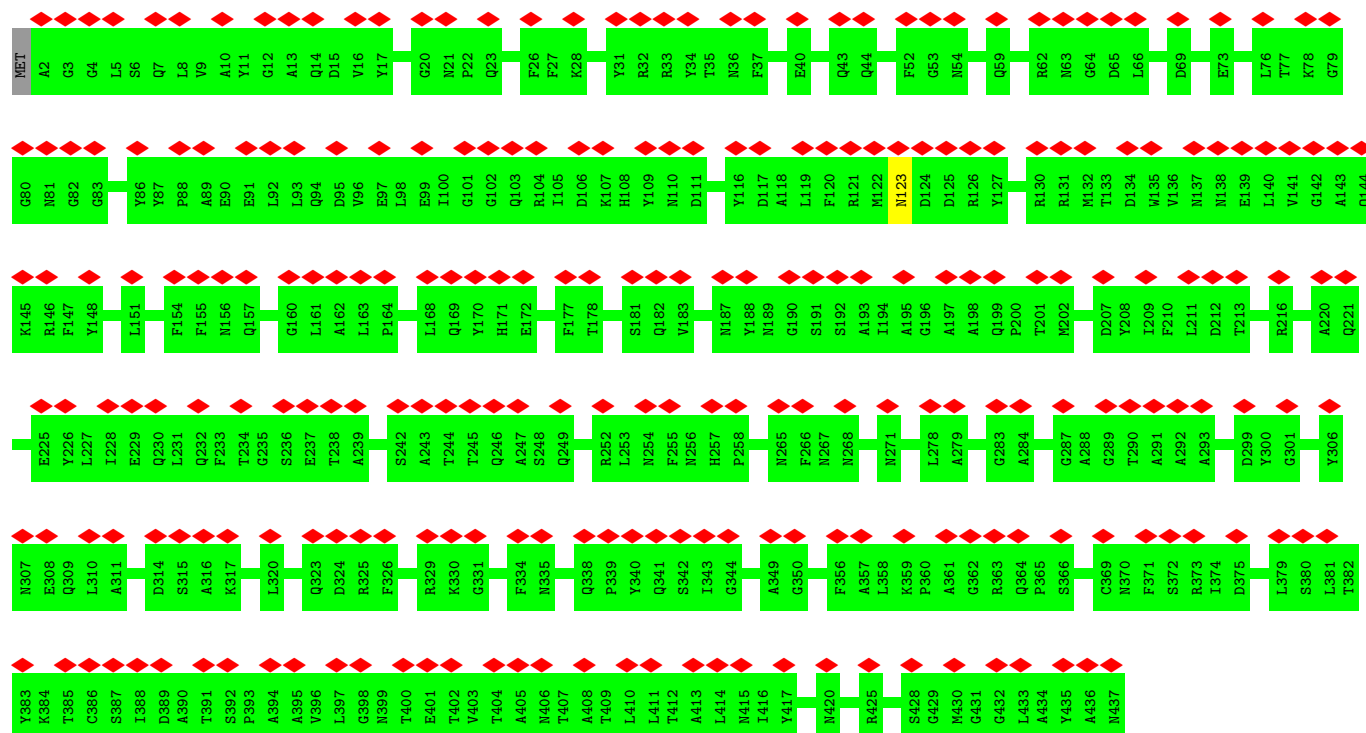


• Molecule 1: Major capsid protein (MCP)

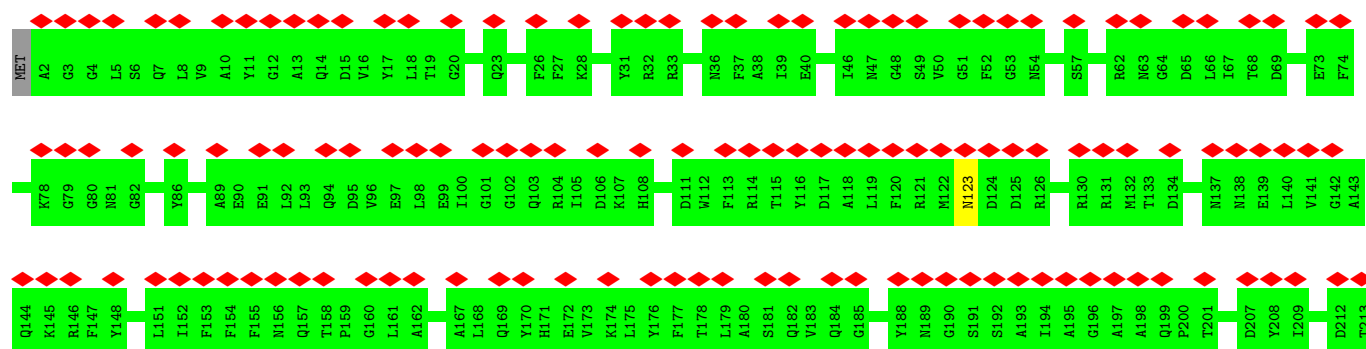


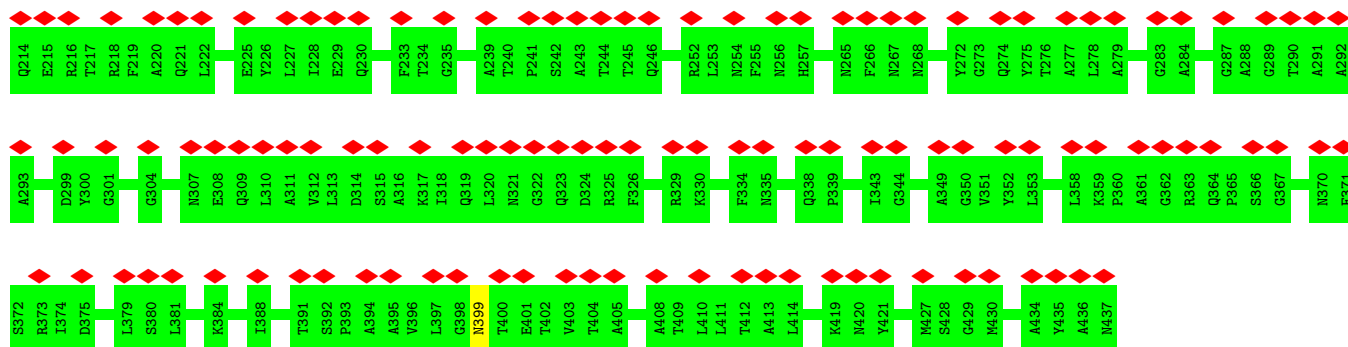


• Molecule 1: Major capsid protein (MCP)

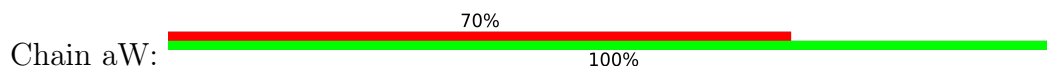


• Molecule 1: Major capsid protein (MCP)



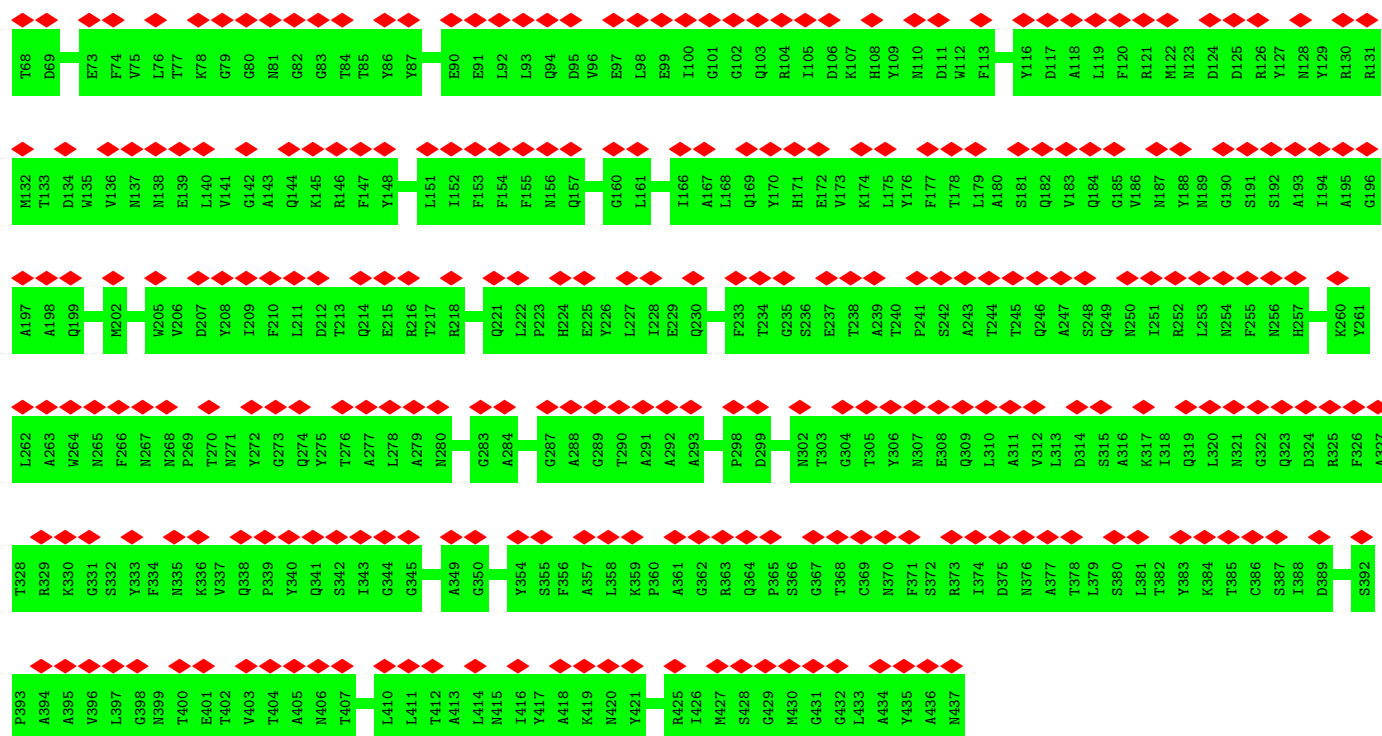


• Molecule 1: Major capsid protein (MCP)

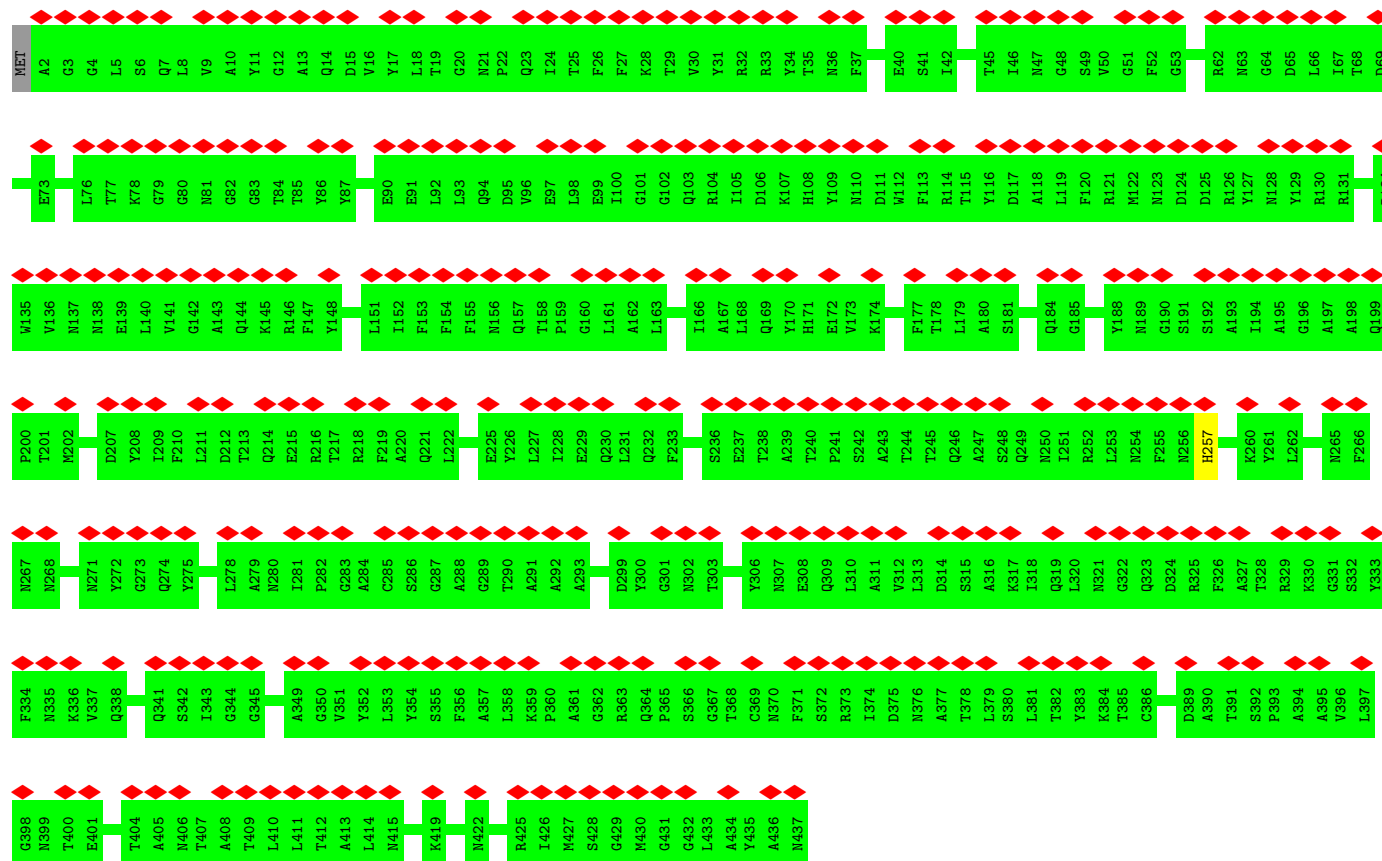
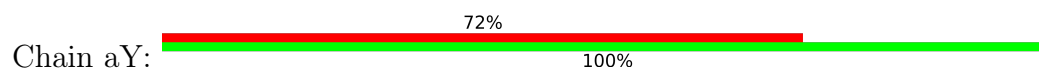


• Molecule 1: Major capsid protein (MCP)

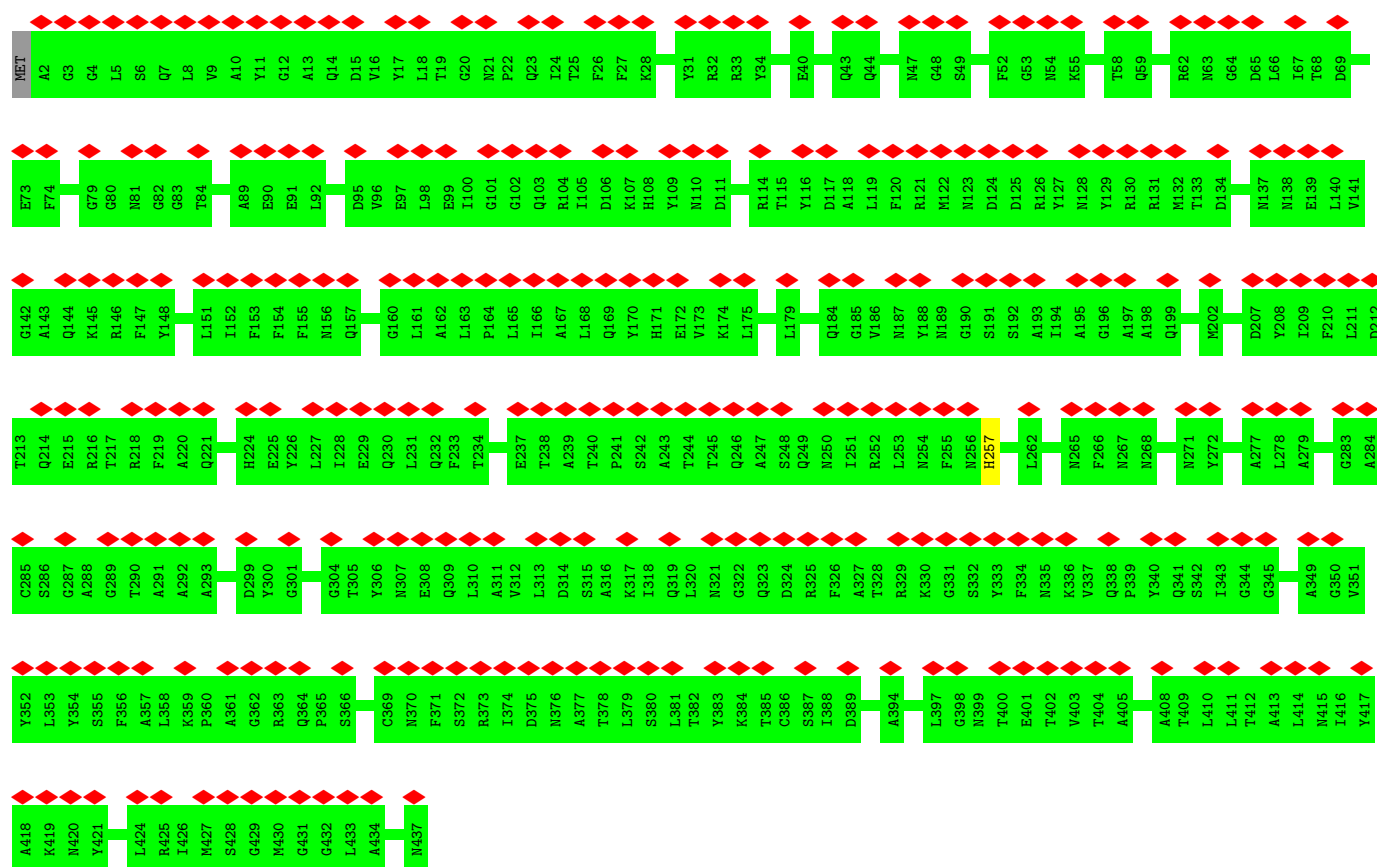




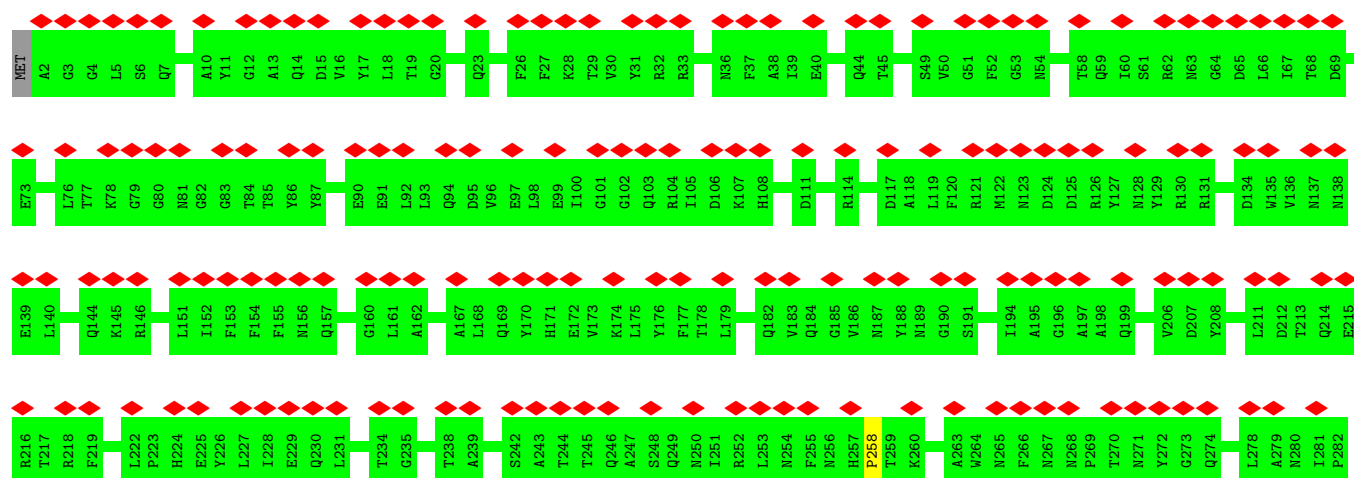
• Molecule 1: Major capsid protein (MCP)

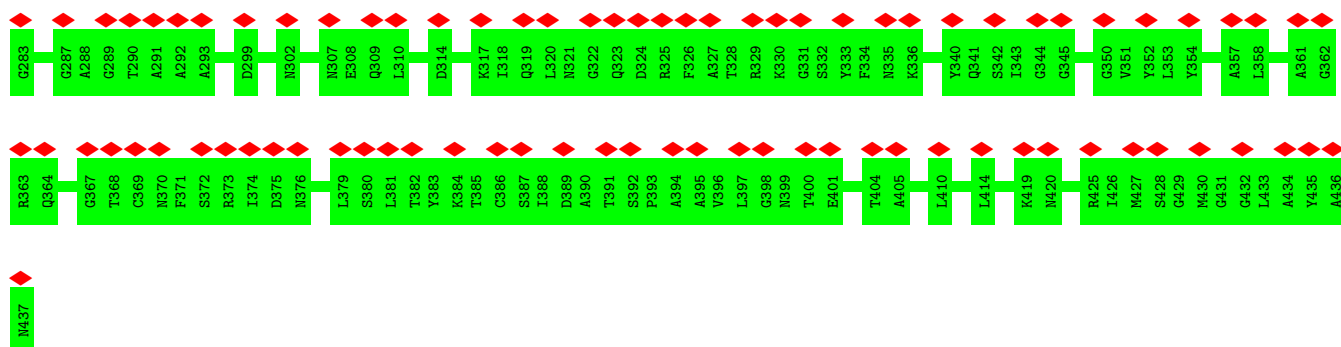


- Molecule 1: Major capsid protein (MCP)

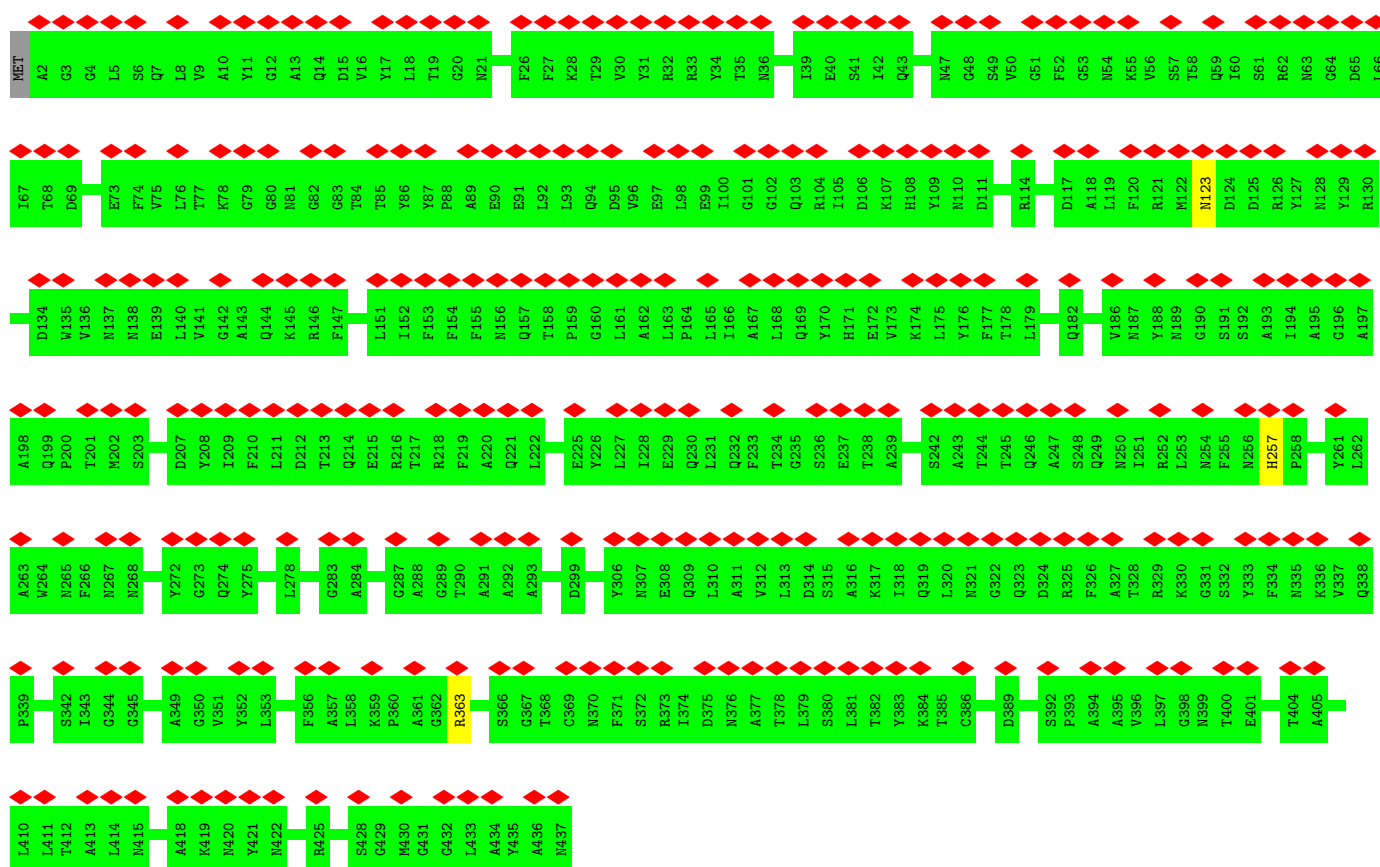


- Molecule 1: Major capsid protein (MCP)

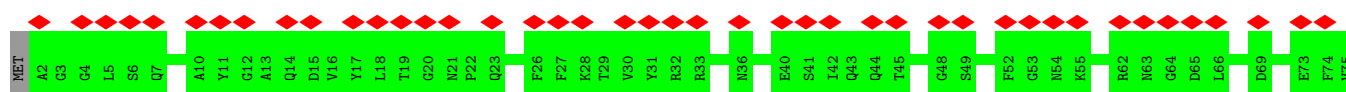


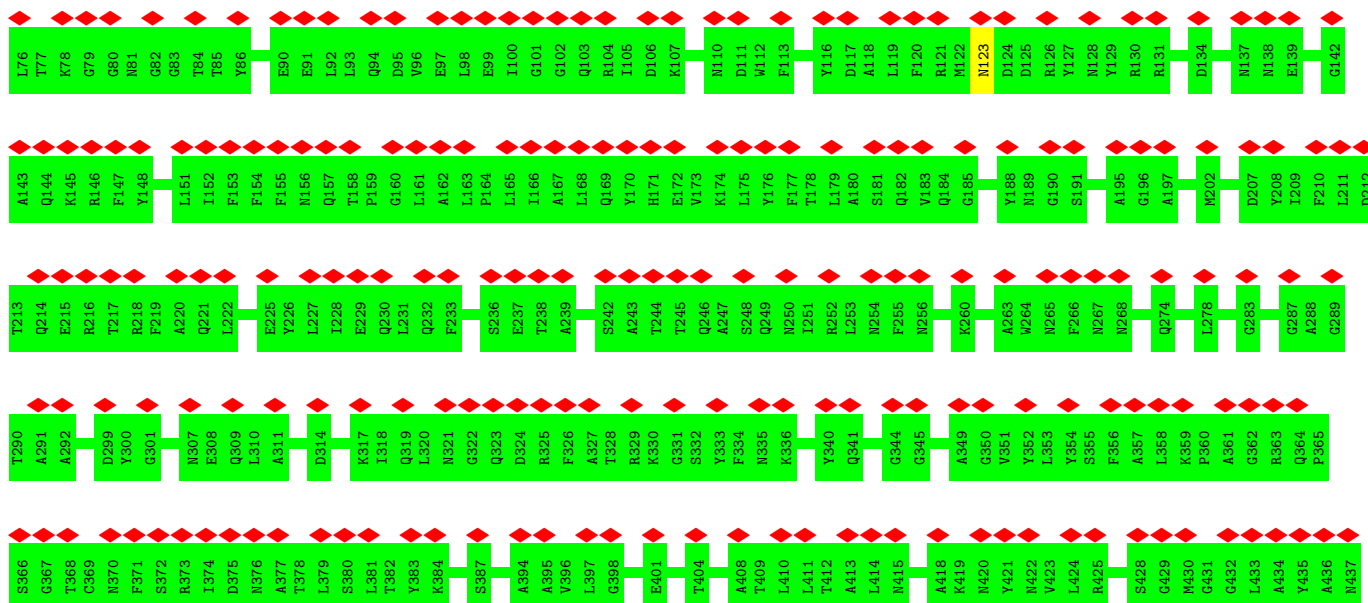


• Molecule 1: Major capsid protein (MCP)

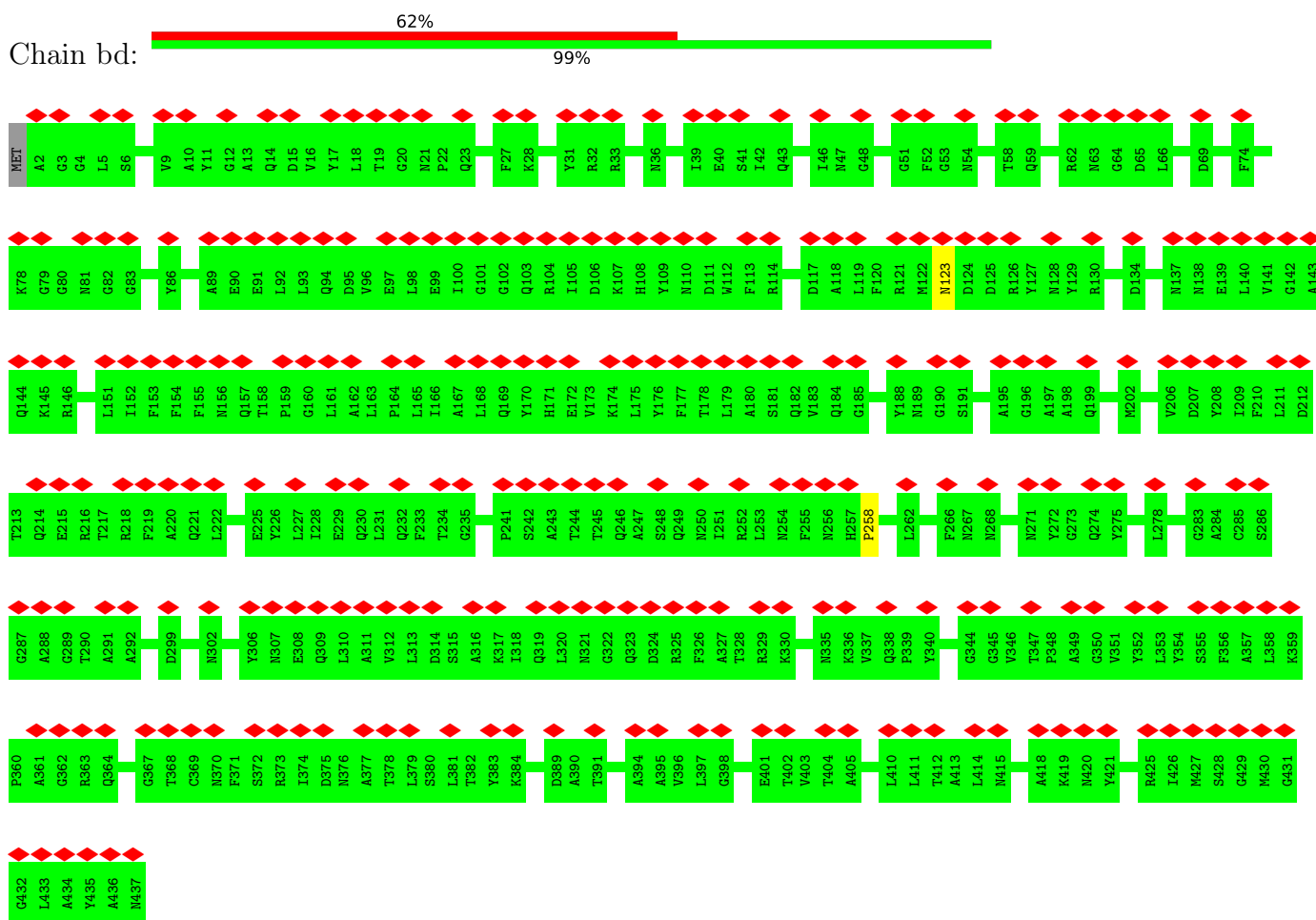


• Molecule 1: Major capsid protein (MCP)

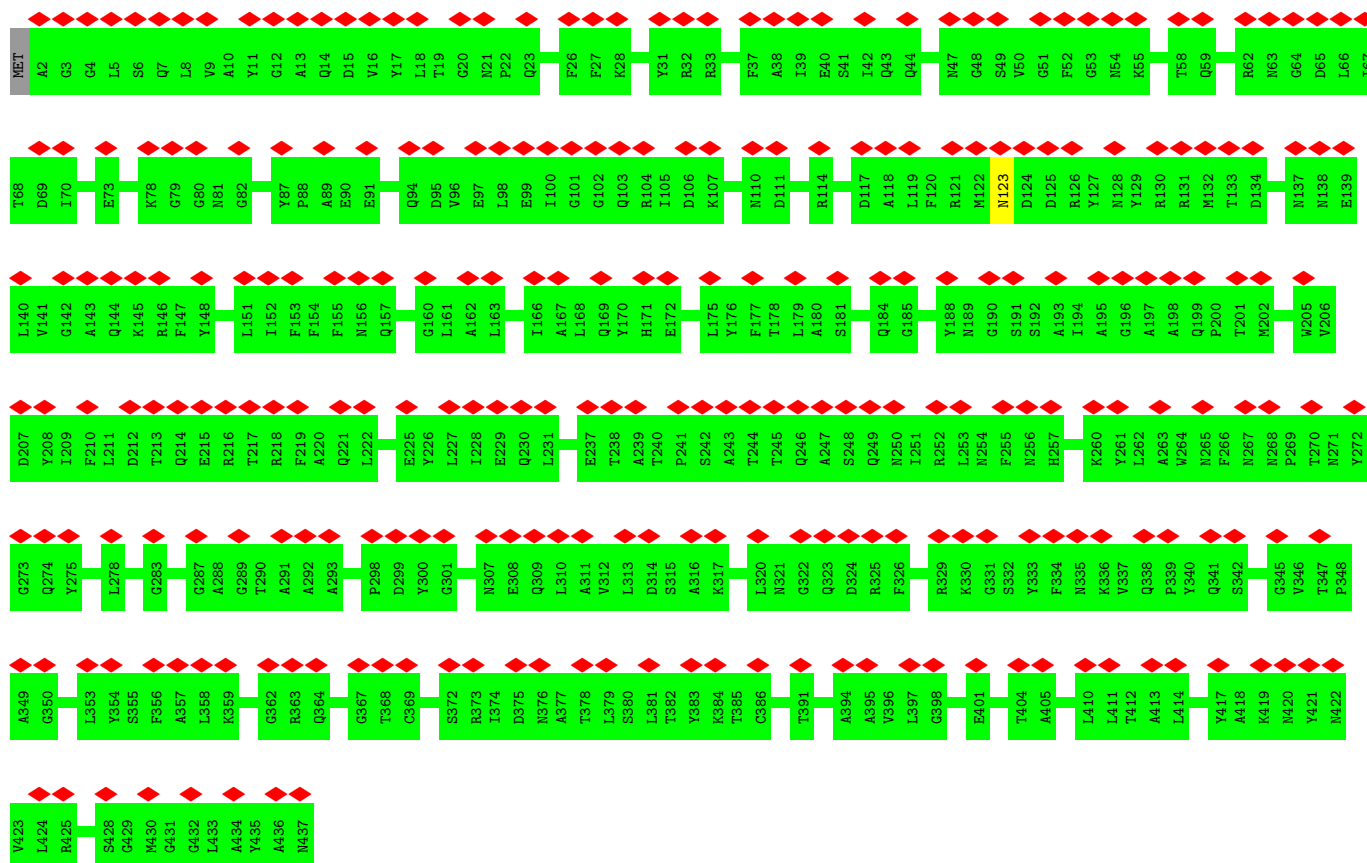




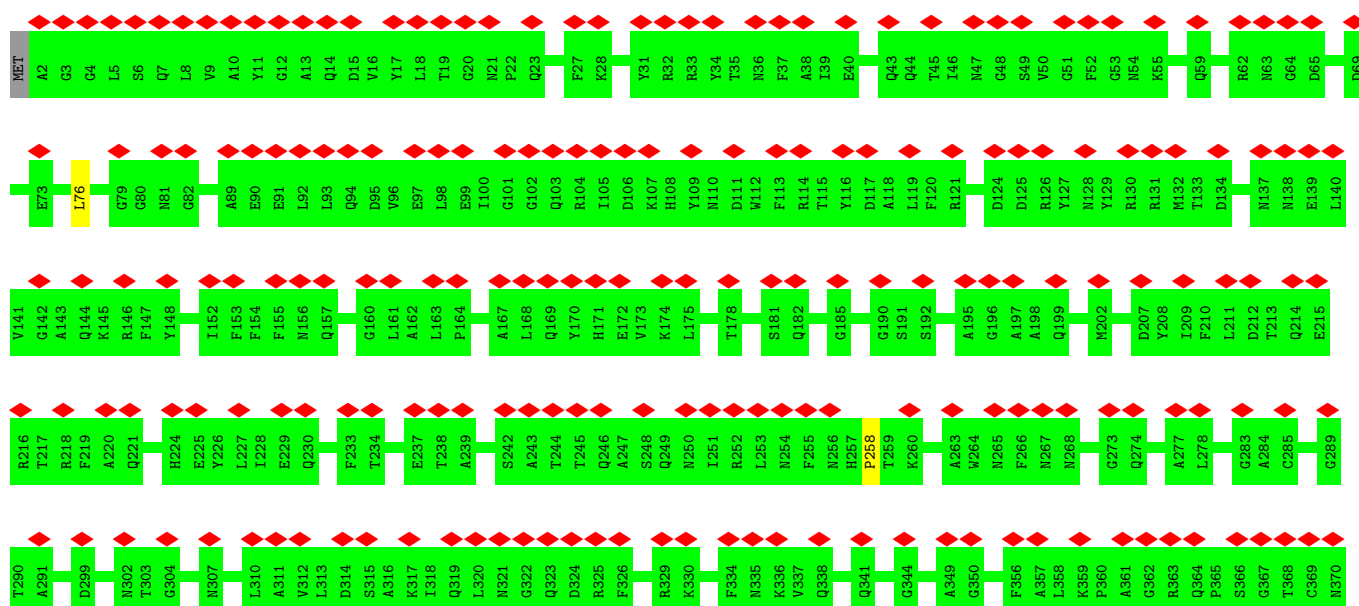
- Molecule 1: Major capsid protein (MCP)

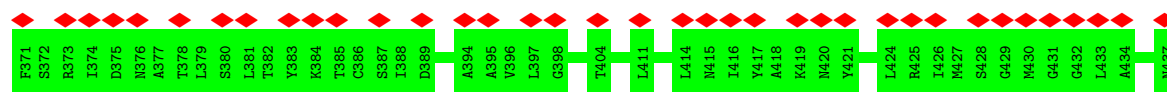


- Molecule 1: Major capsid protein (MCP)

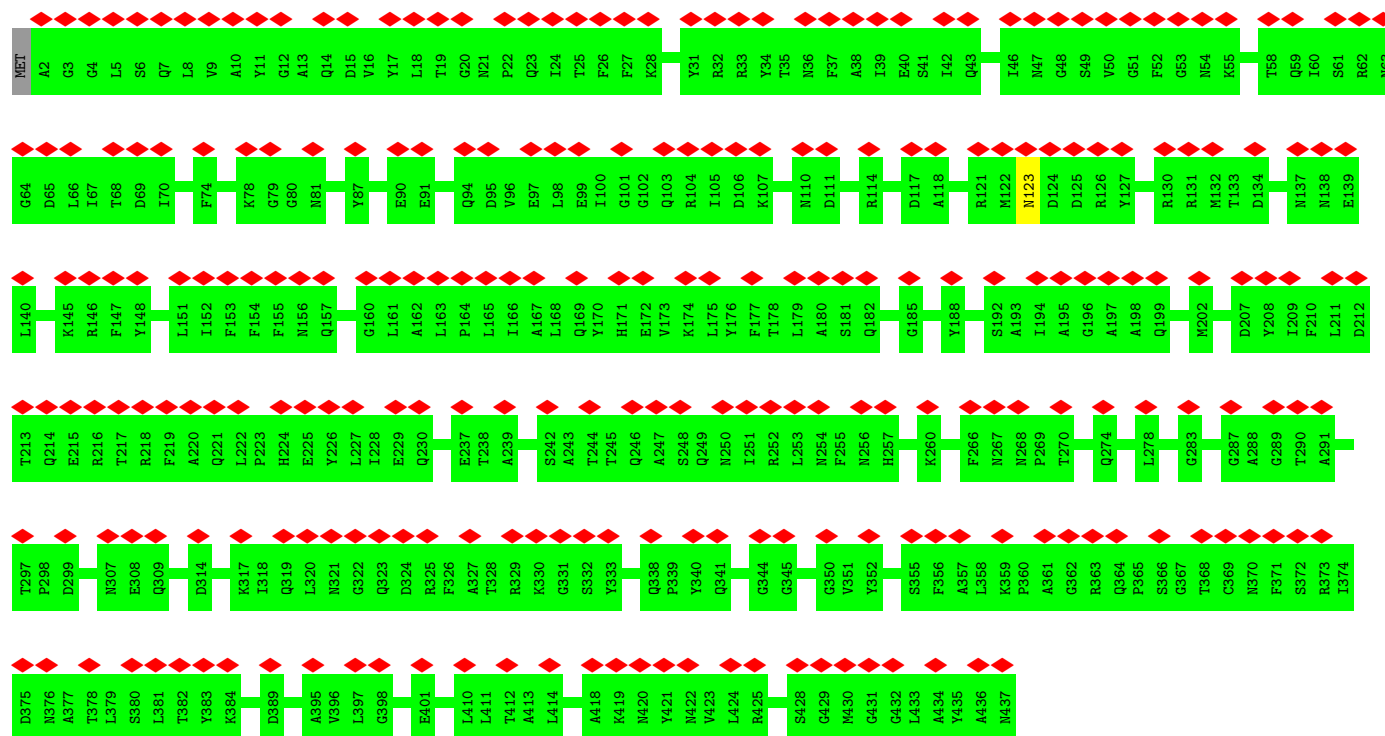


• Molecule 1: Major capsid protein (MCP)

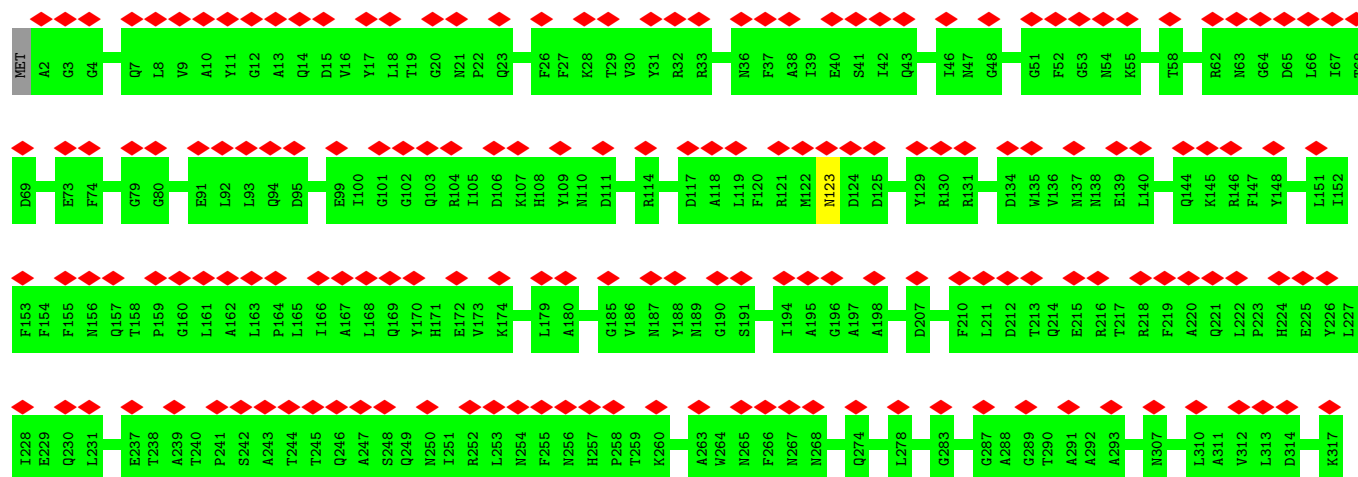


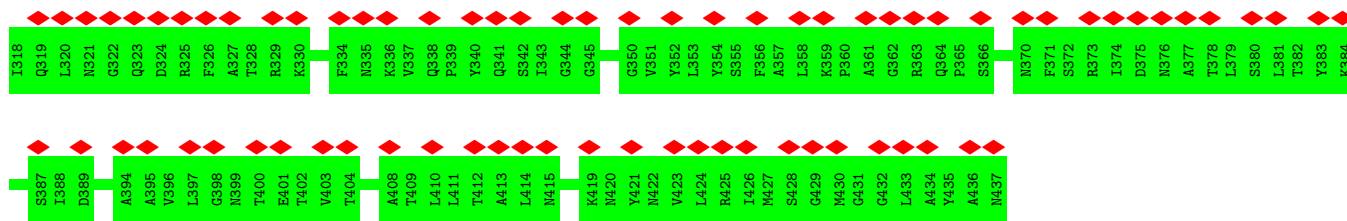


• Molecule 1: Major capsid protein (MCP)

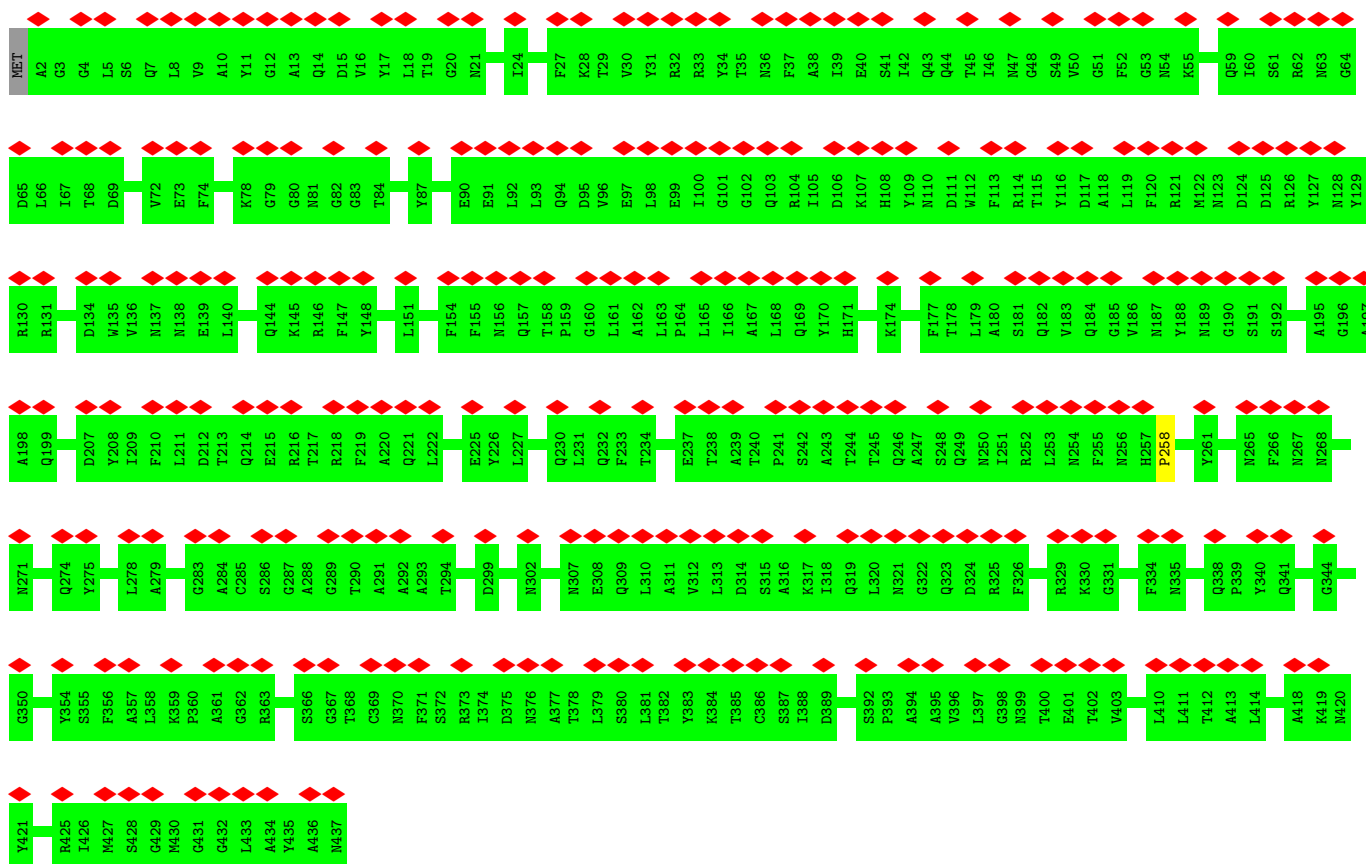


• Molecule 1: Major capsid protein (MCP)

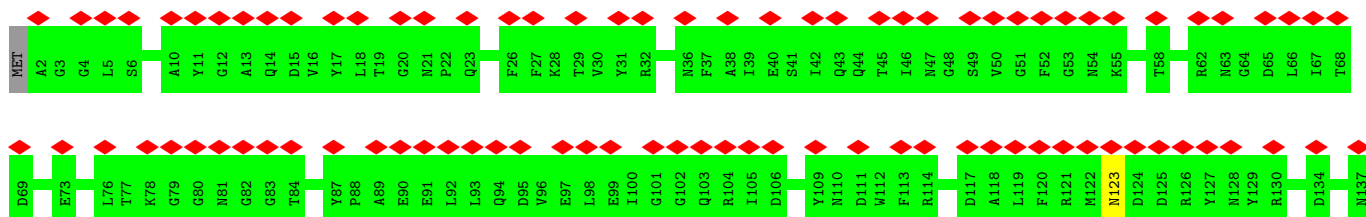


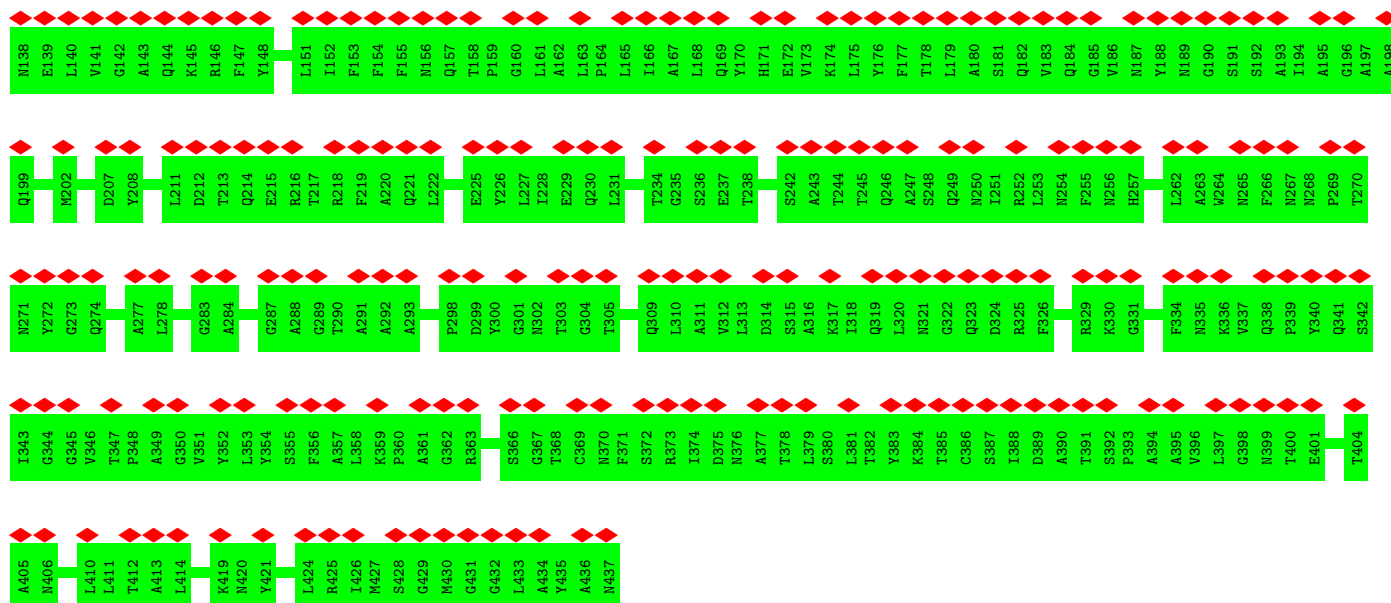


• Molecule 1: Major capsid protein (MCP)

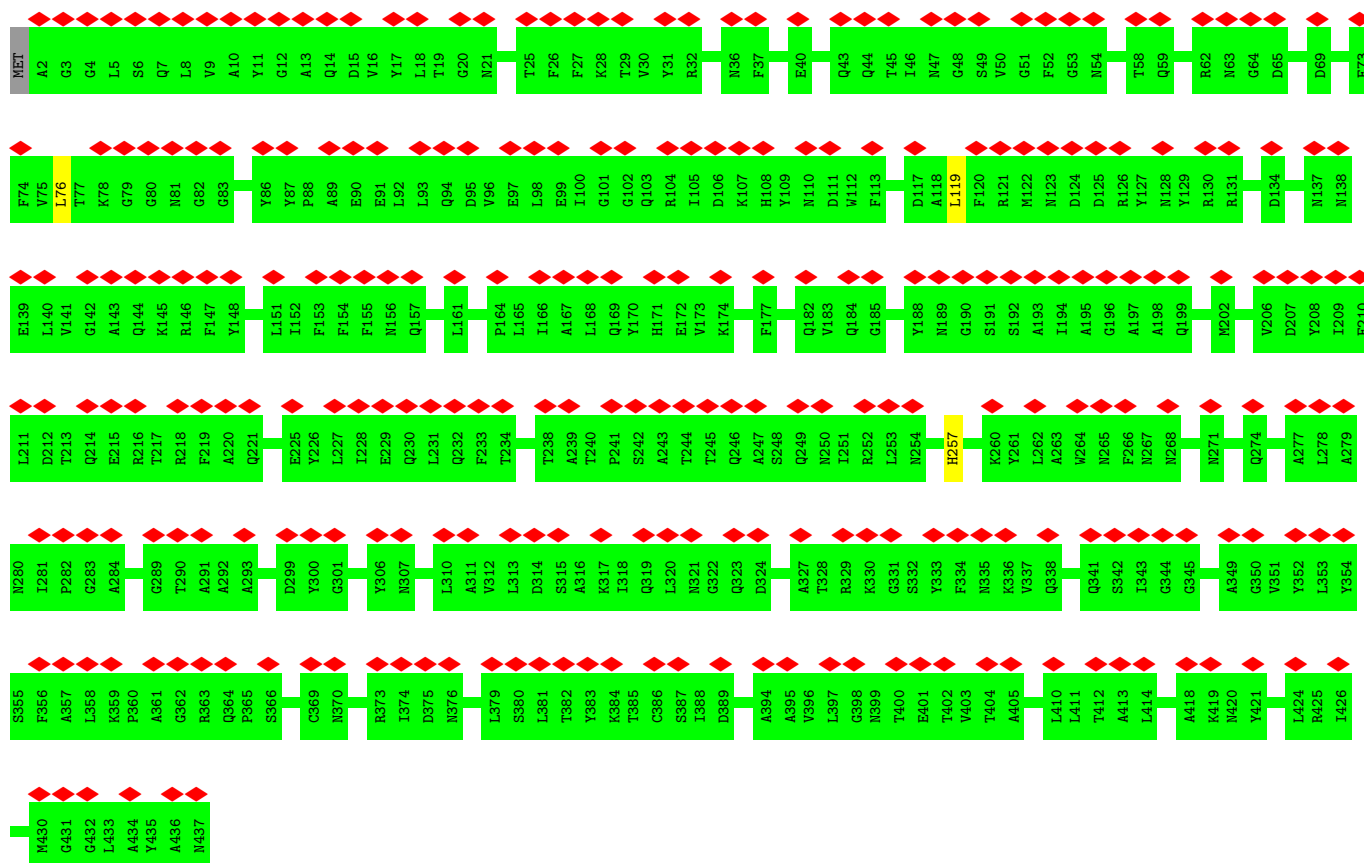


• Molecule 1: Major capsid protein (MCP)

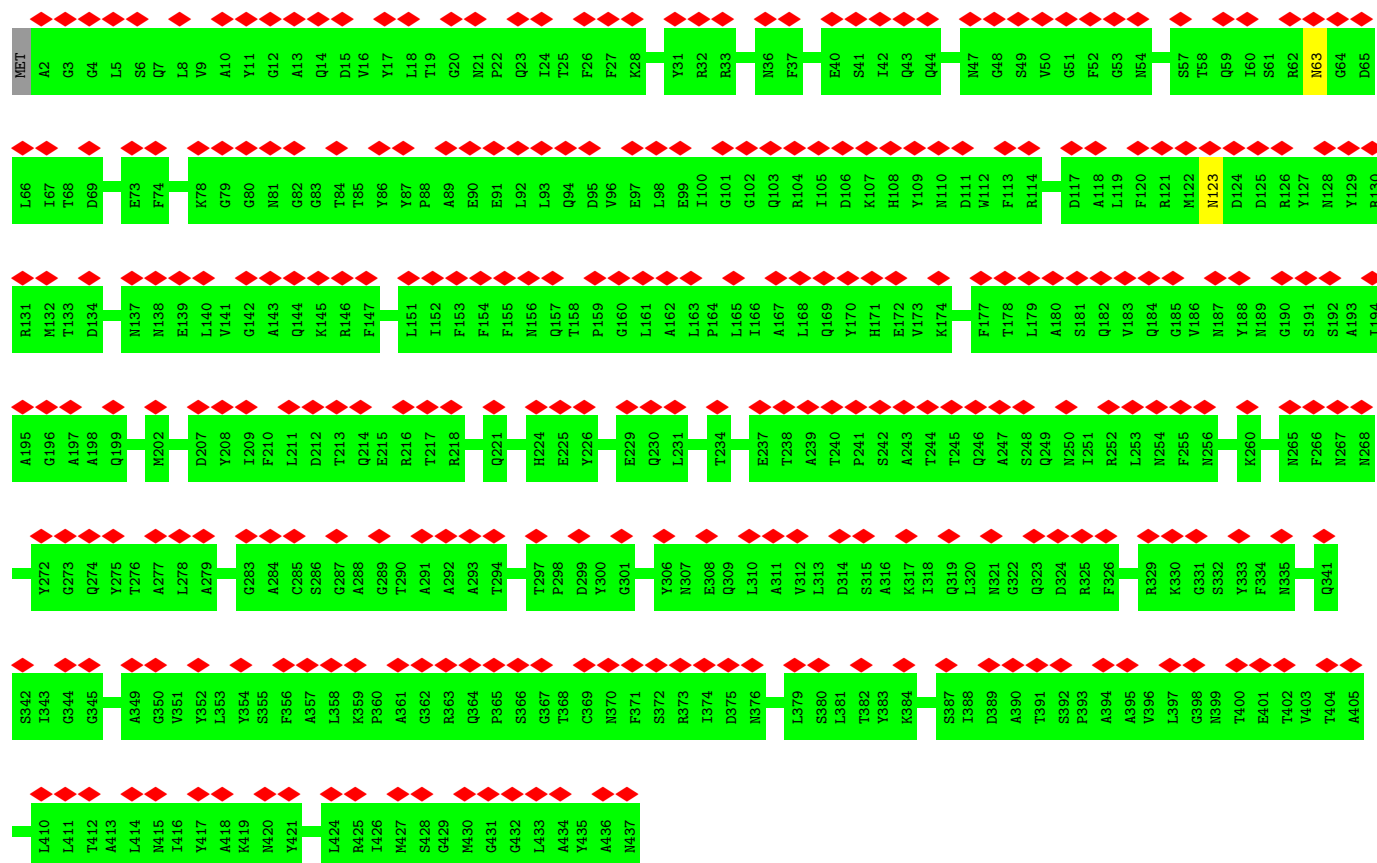




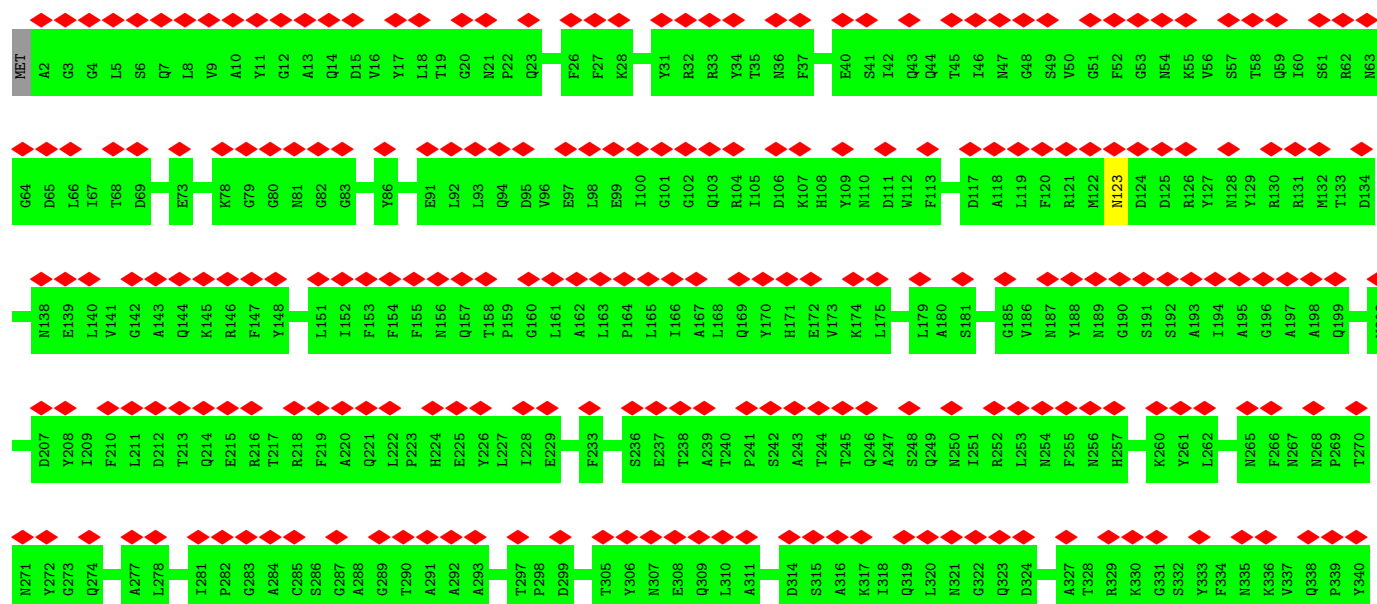
• Molecule 1: Major capsid protein (MCP)

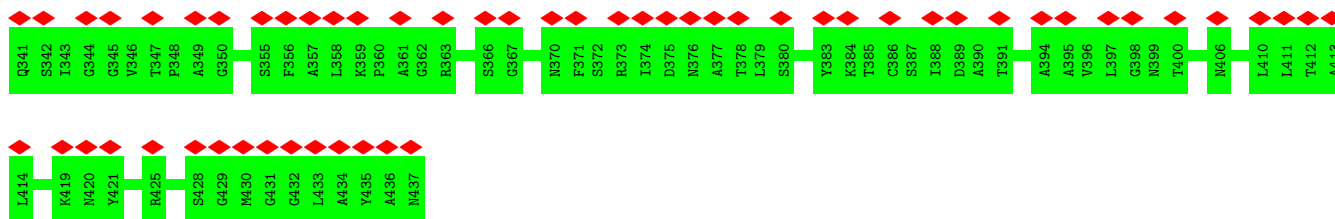


• Molecule 1: Major capsid protein (MCP)

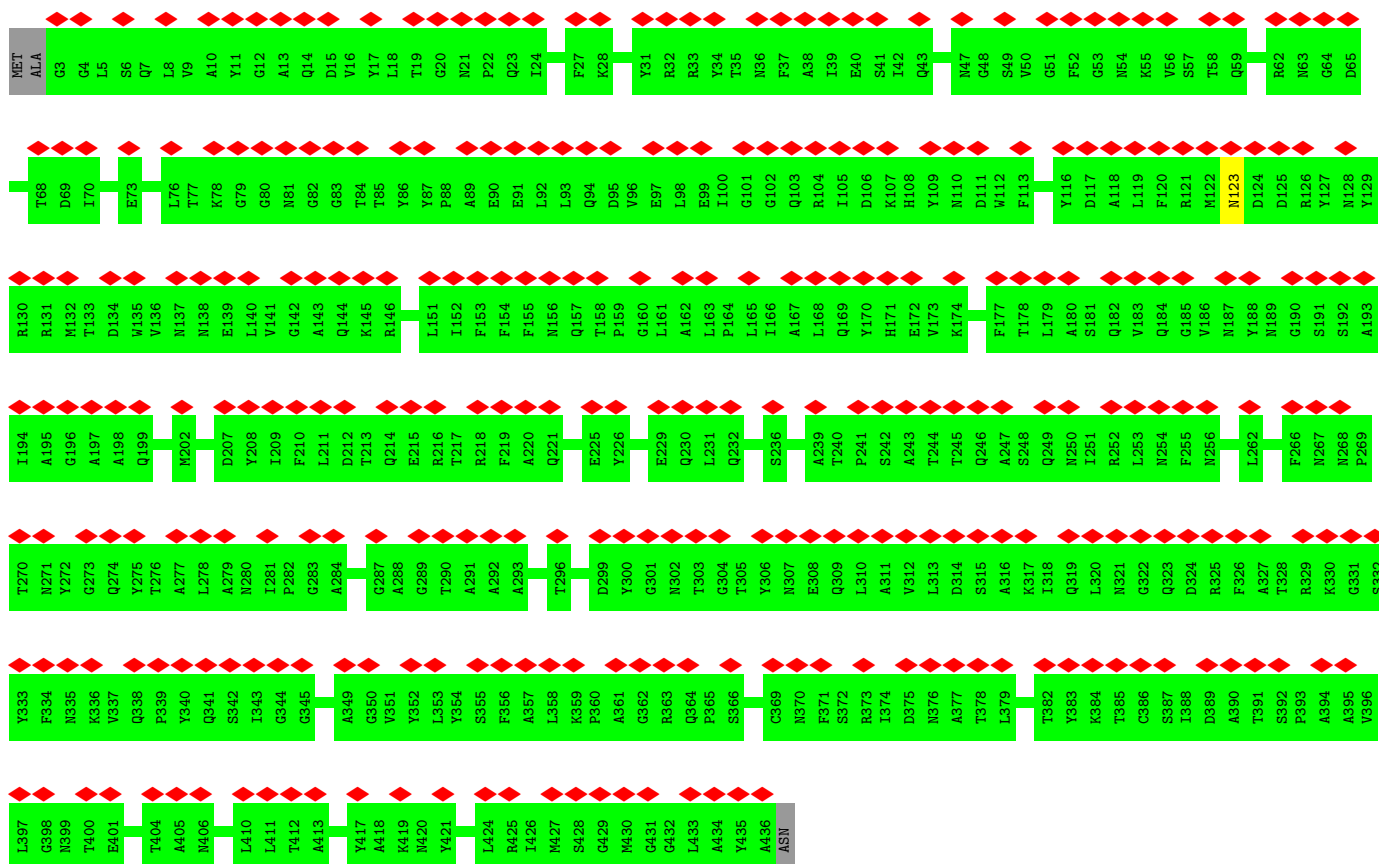


• Molecule 1: Major capsid protein (MCP)

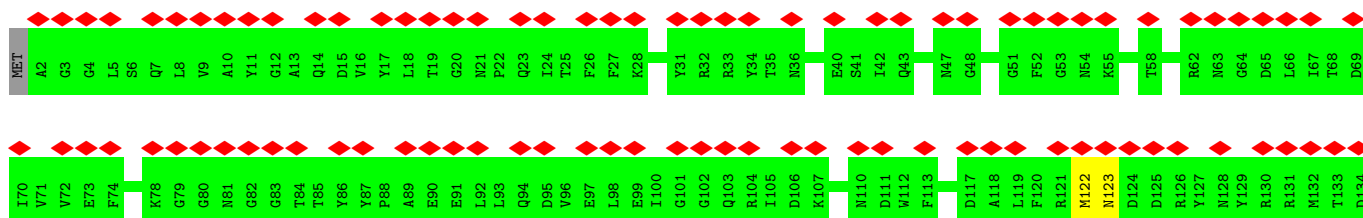


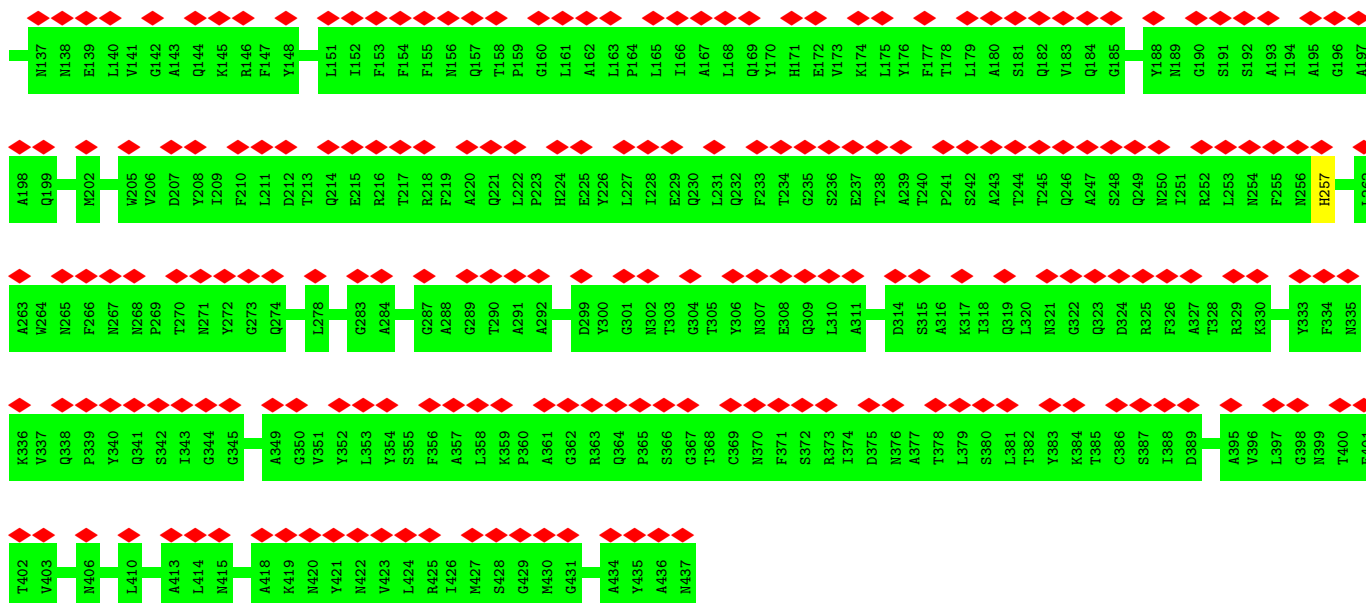


• Molecule 1: Major capsid protein (MCP)

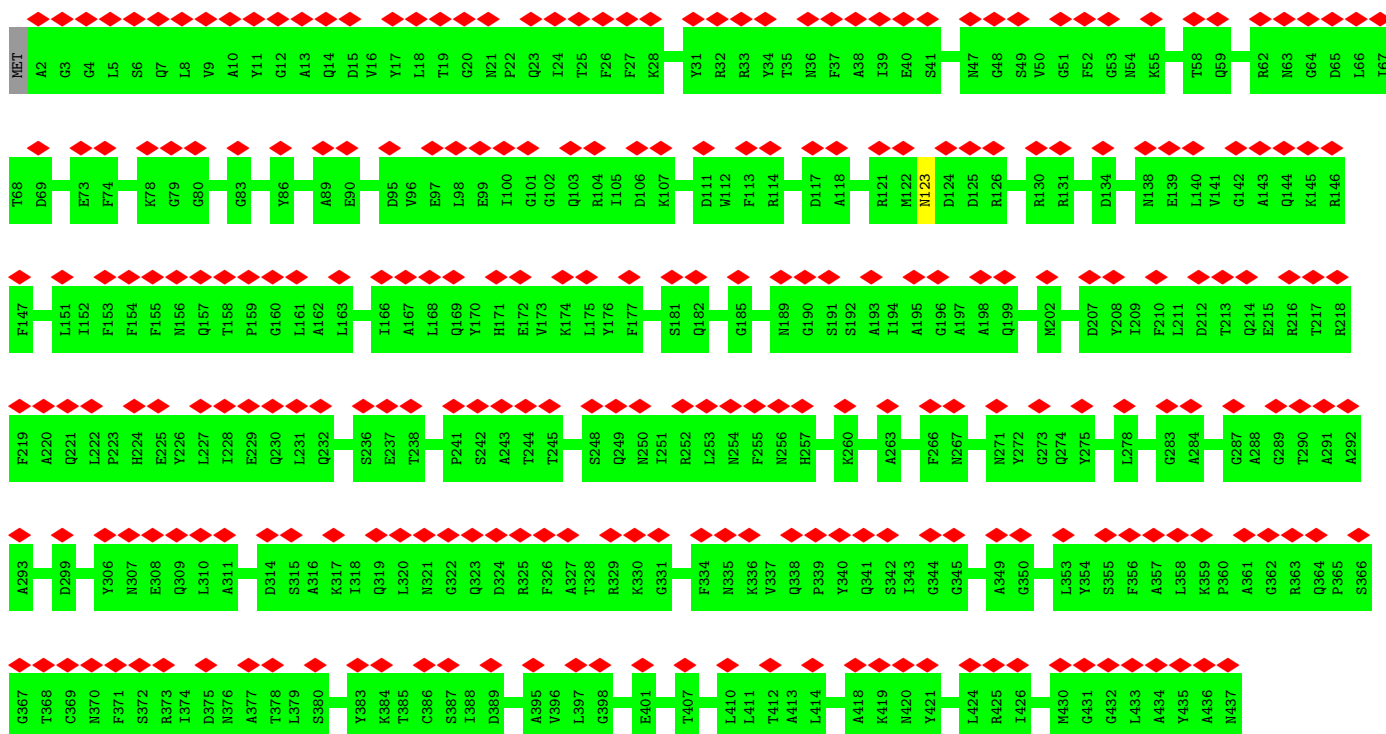


• Molecule 1: Major capsid protein (MCP)



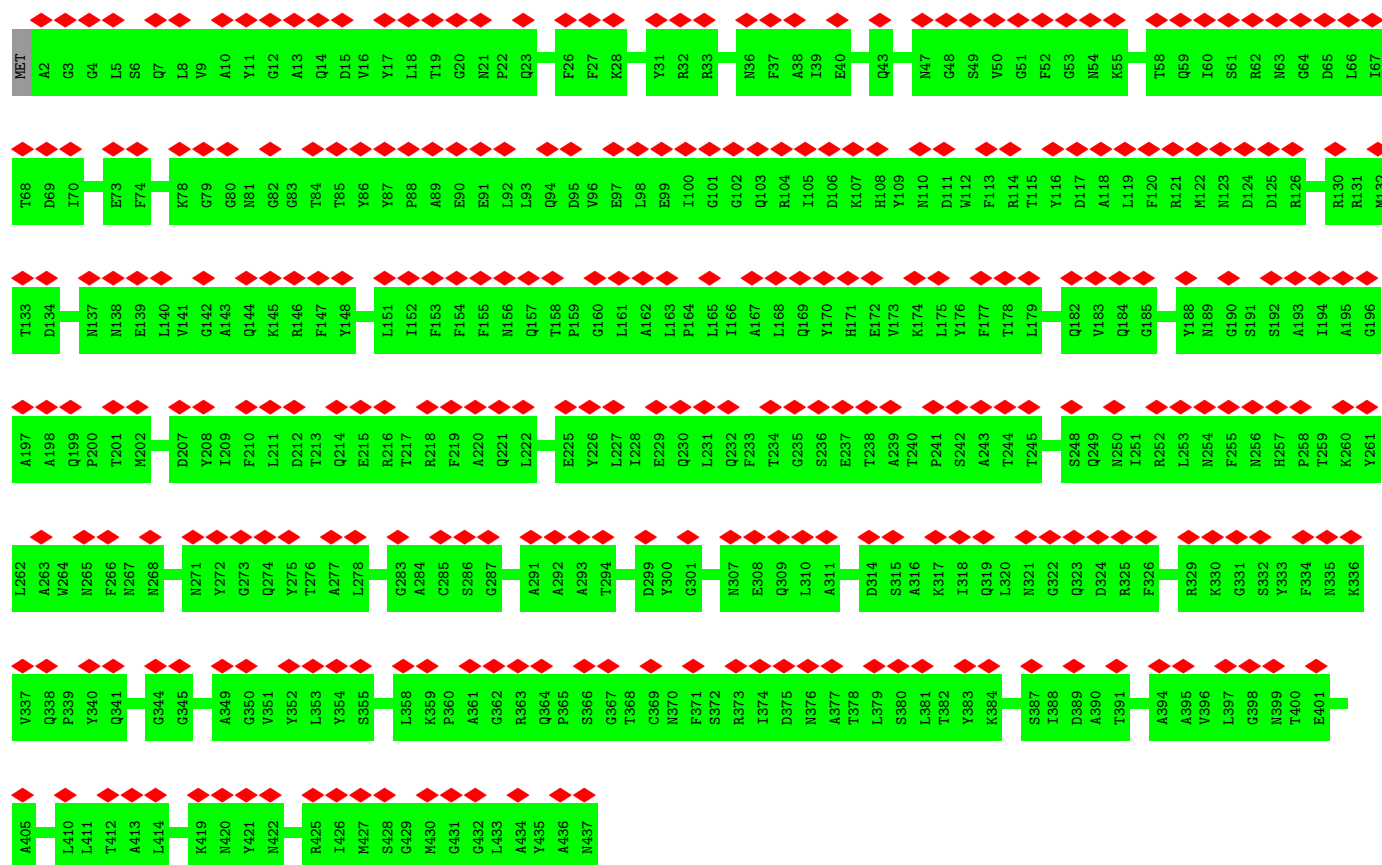


• Molecule 1: Major capsid protein (MCP)



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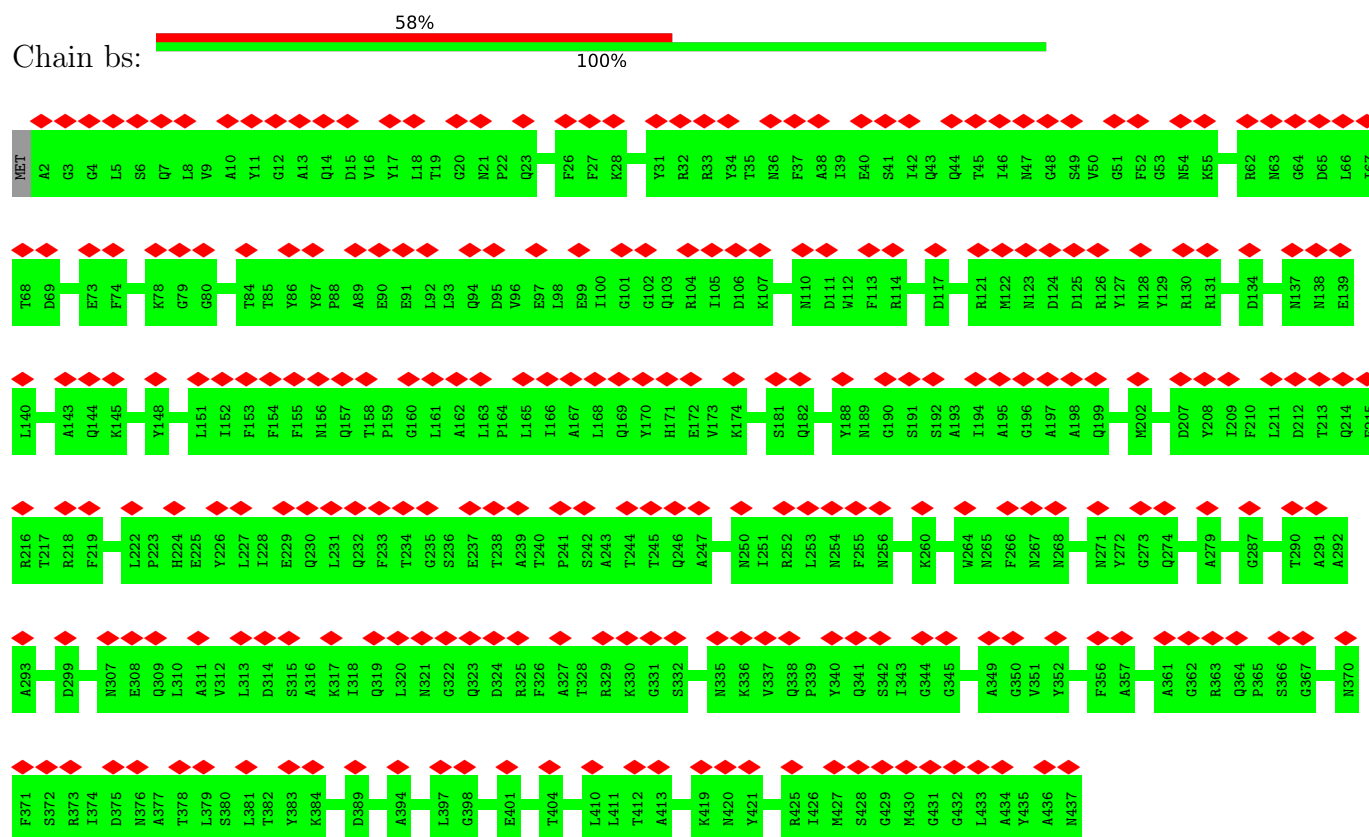




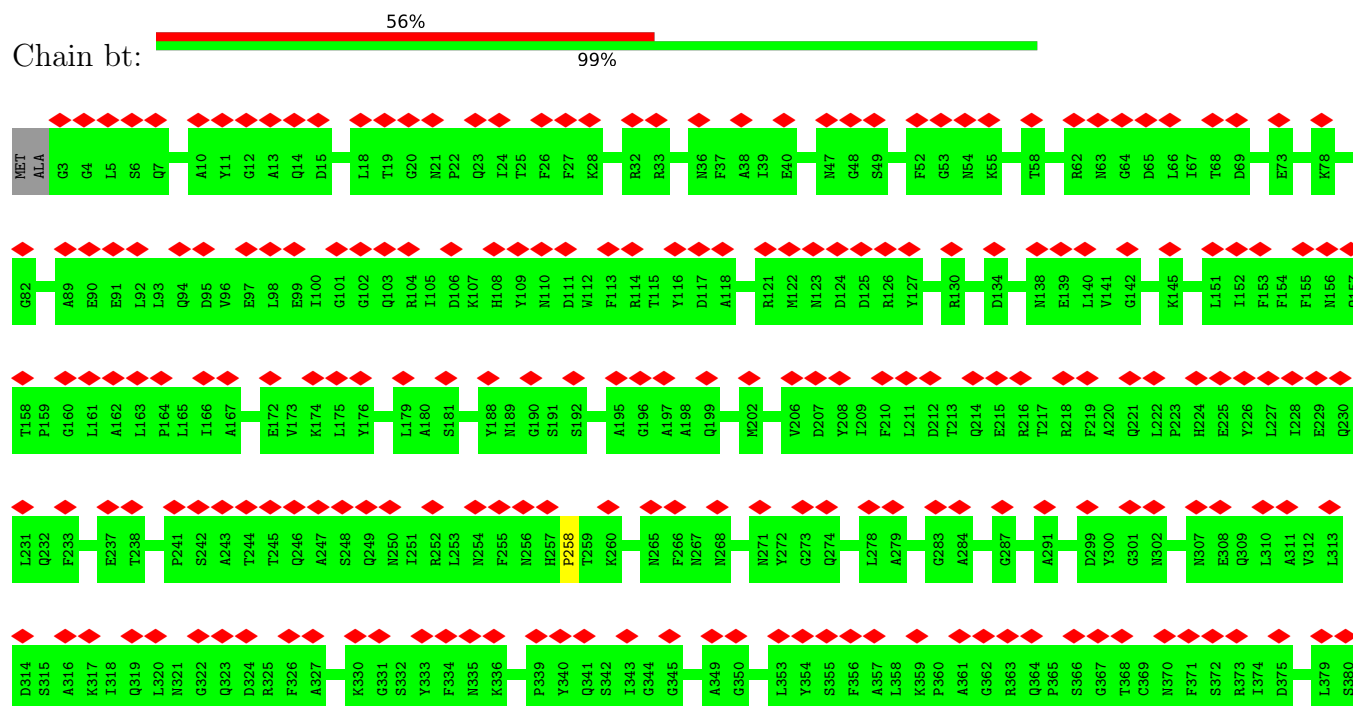
• Molecule 1: Major capsid protein (MCP)

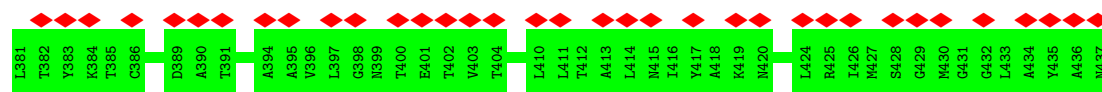


- Molecule 1: Major capsid protein (MCP)

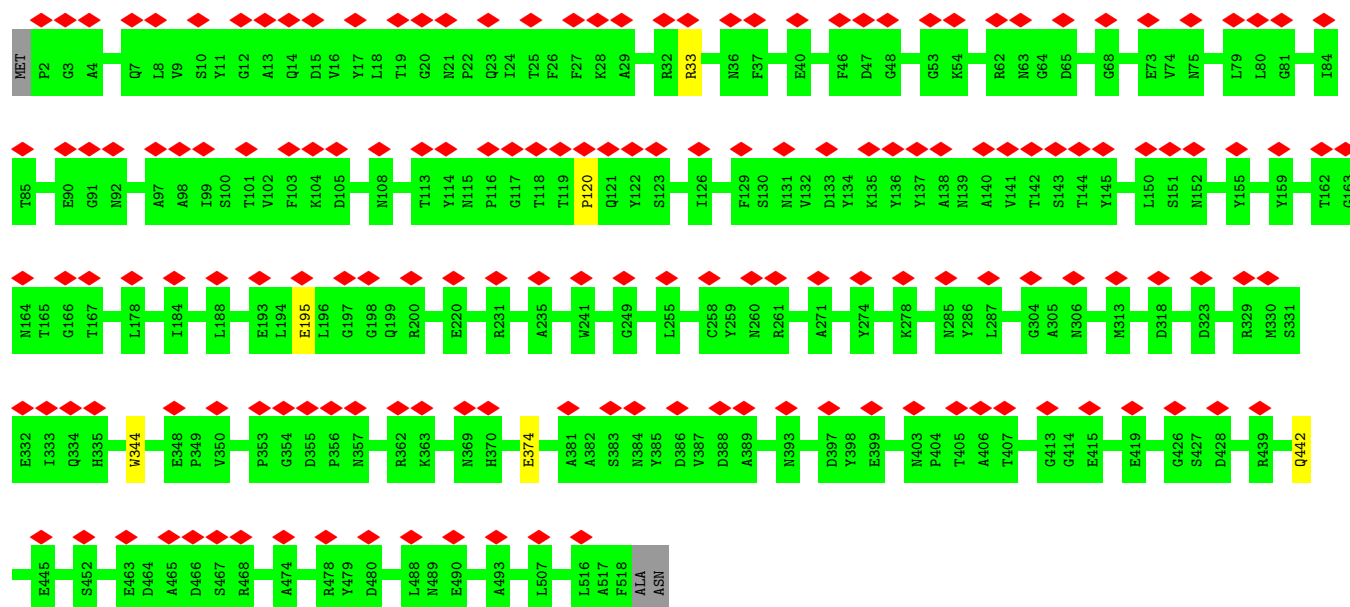


- Molecule 1: Major capsid protein (MCP)

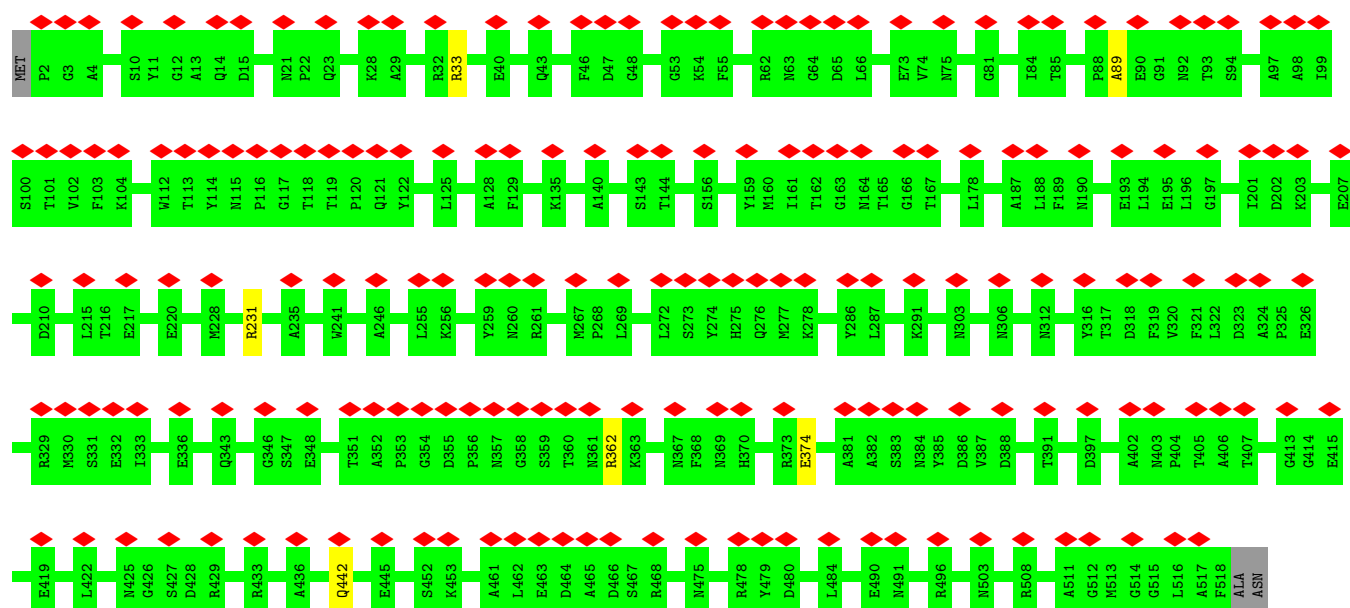




• Molecule 2: MCPv1

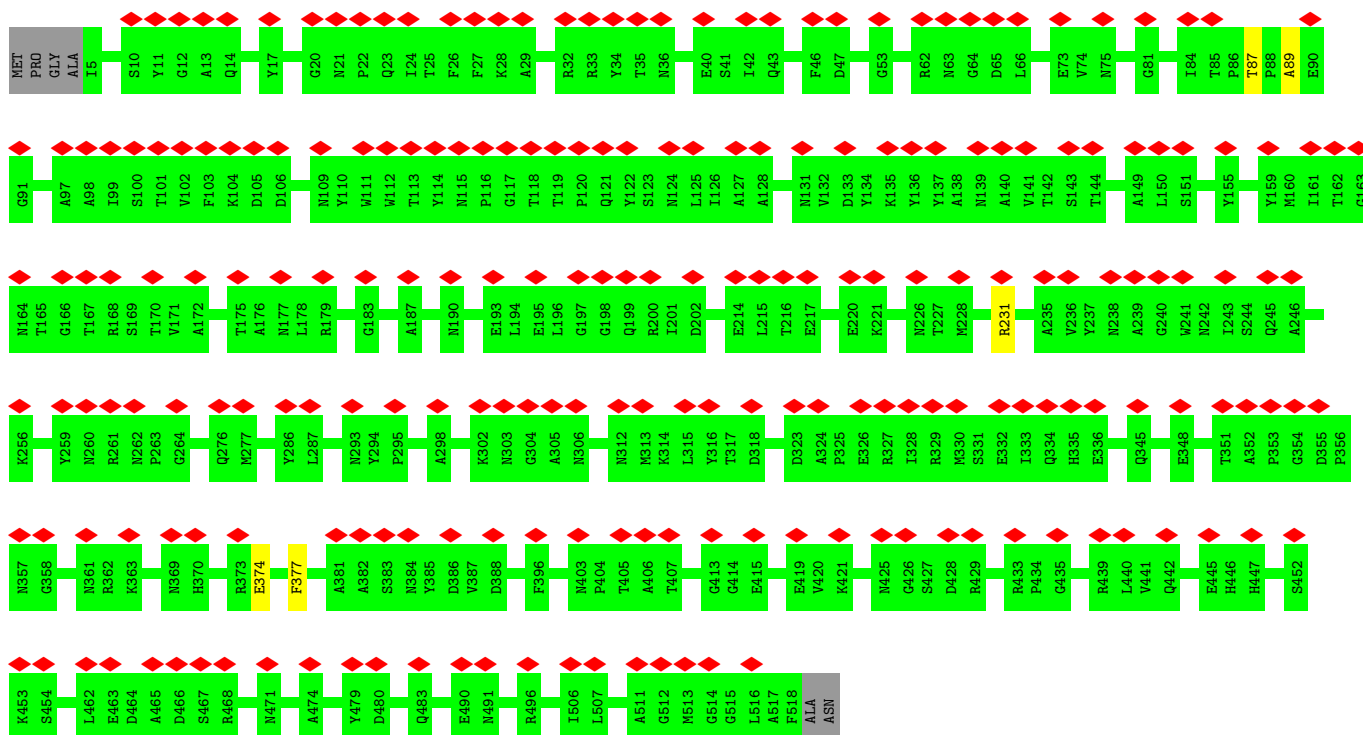
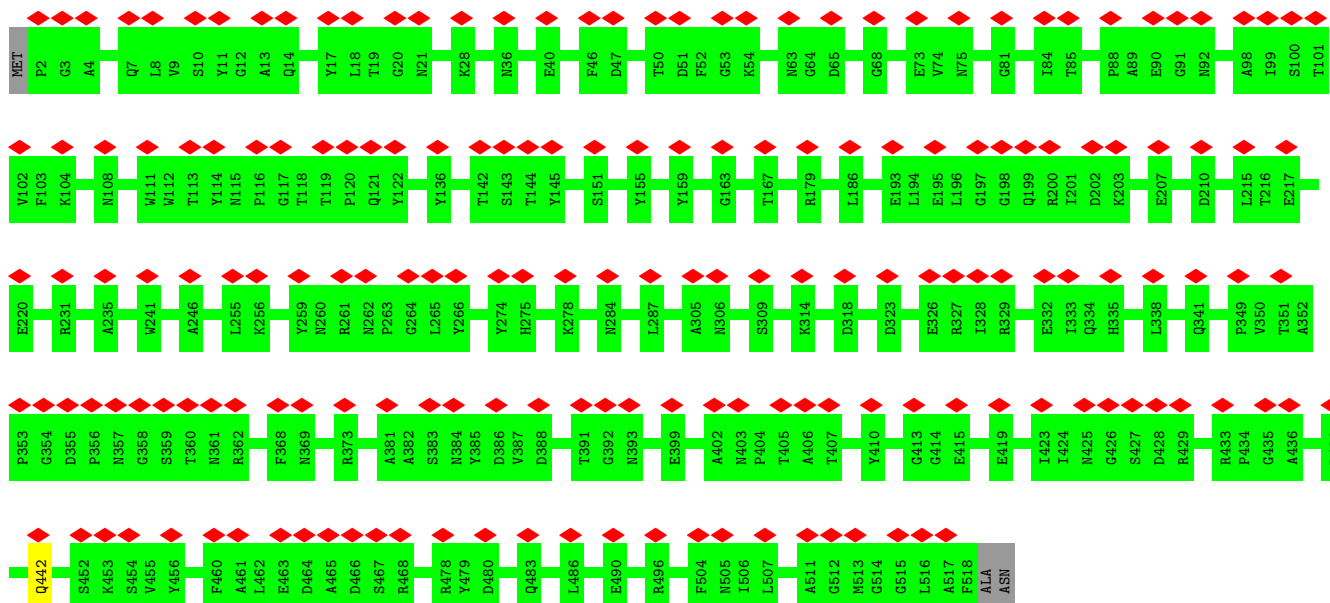


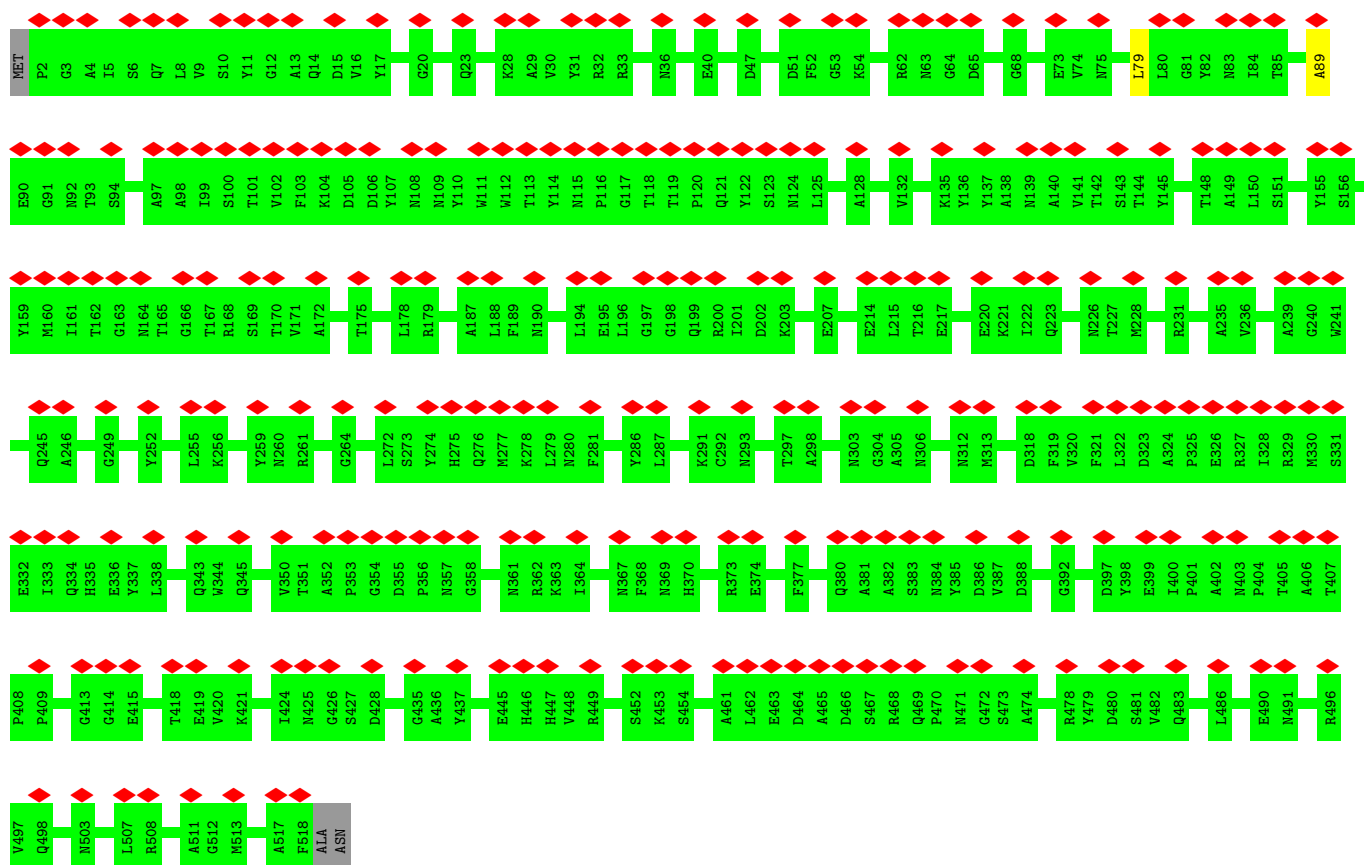
• Molecule 2: MCPv1



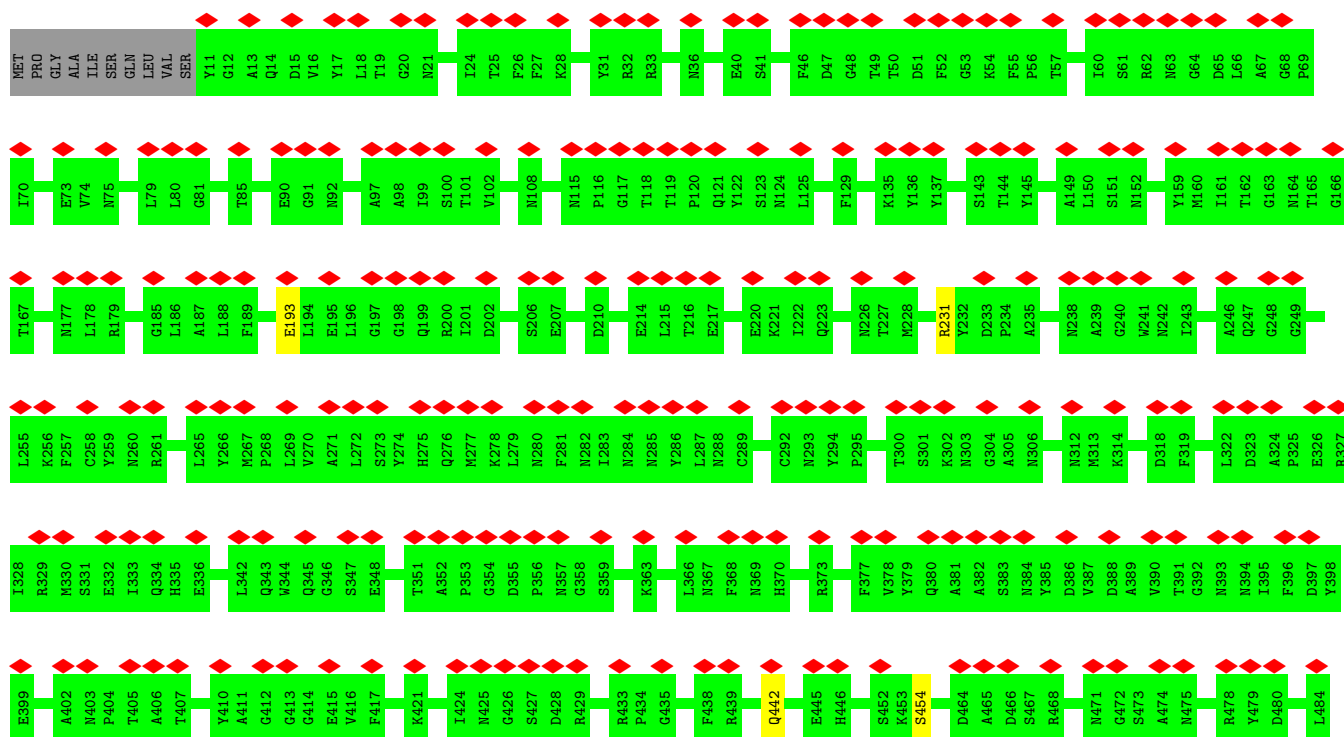
• Molecule 2: MCPv1





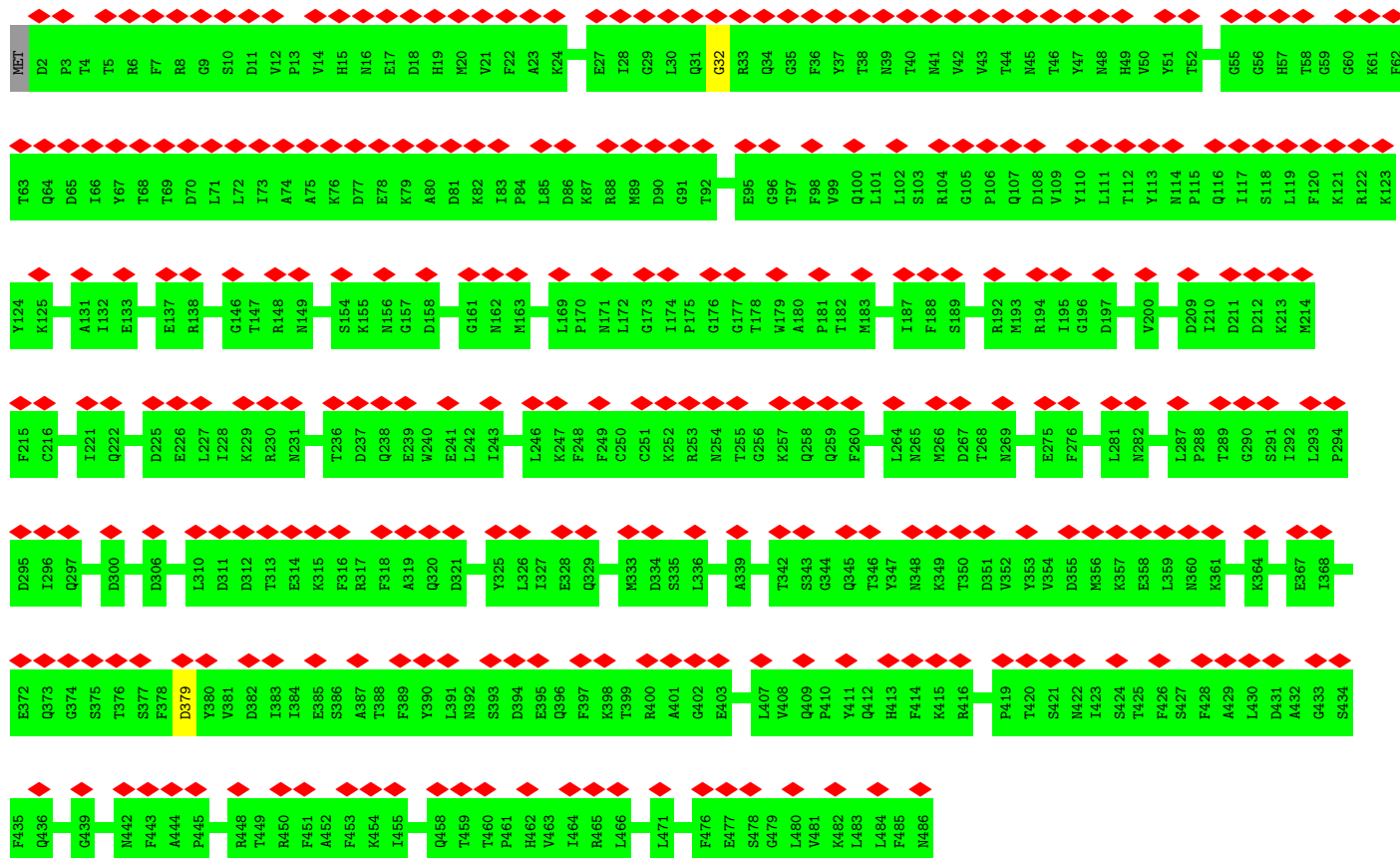


• Molecule 2: MCPv1



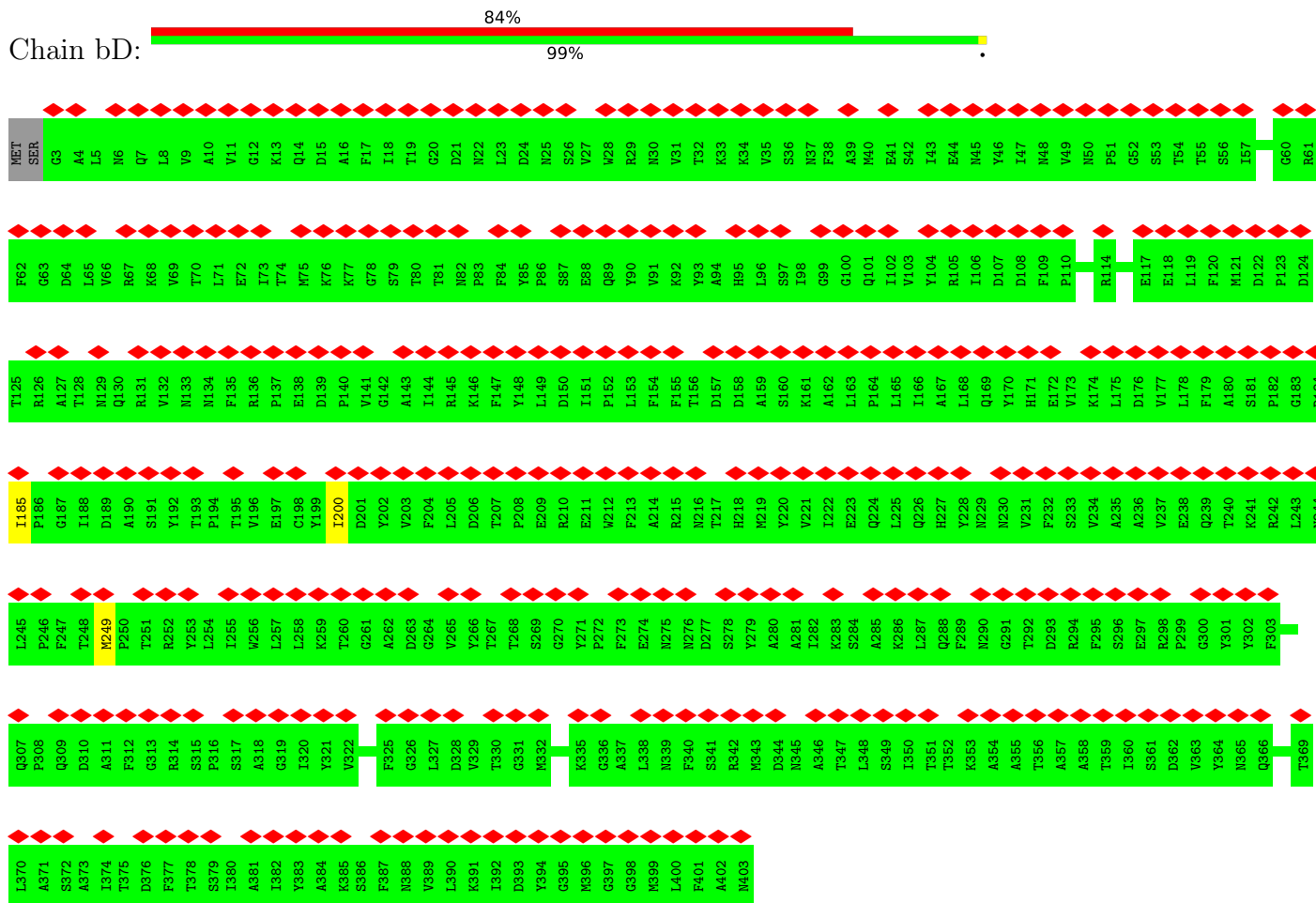


• Molecule 3: MCPv2



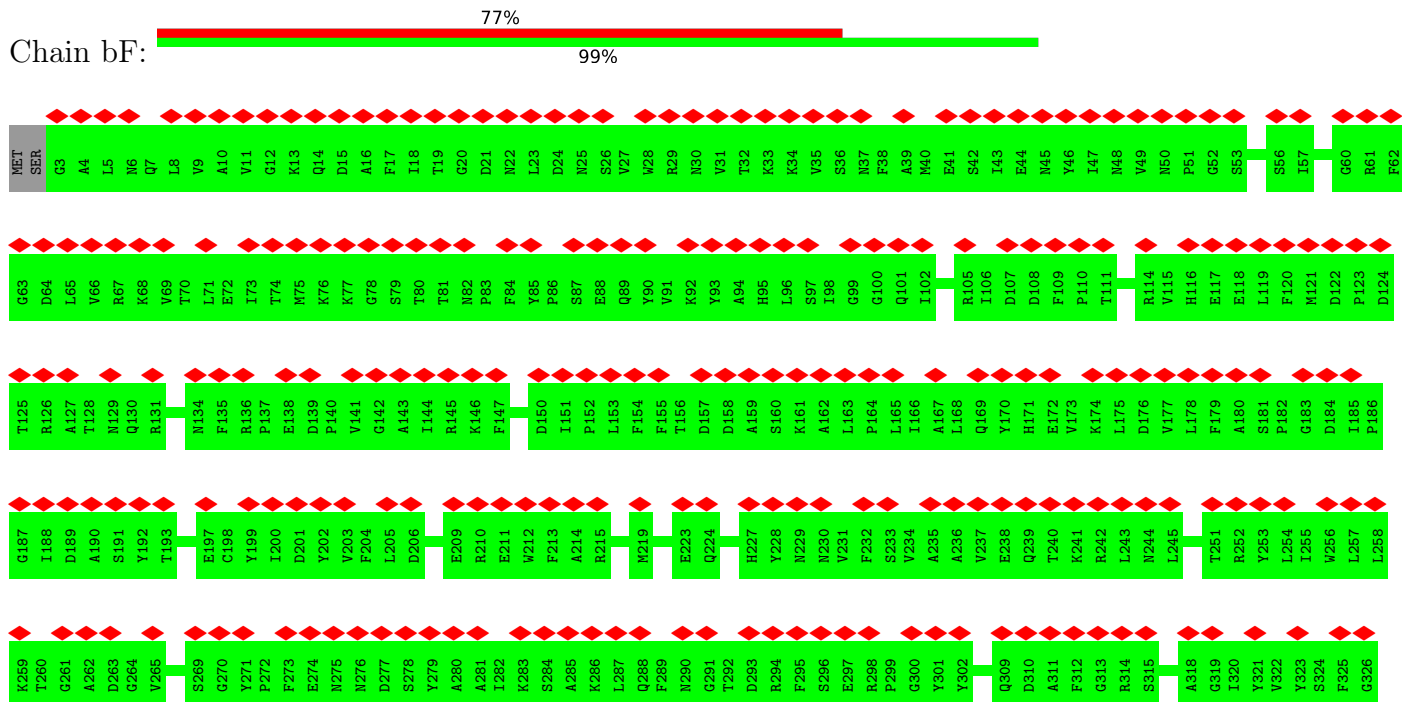
● Molecule 4: MCPv3

Chain bD:



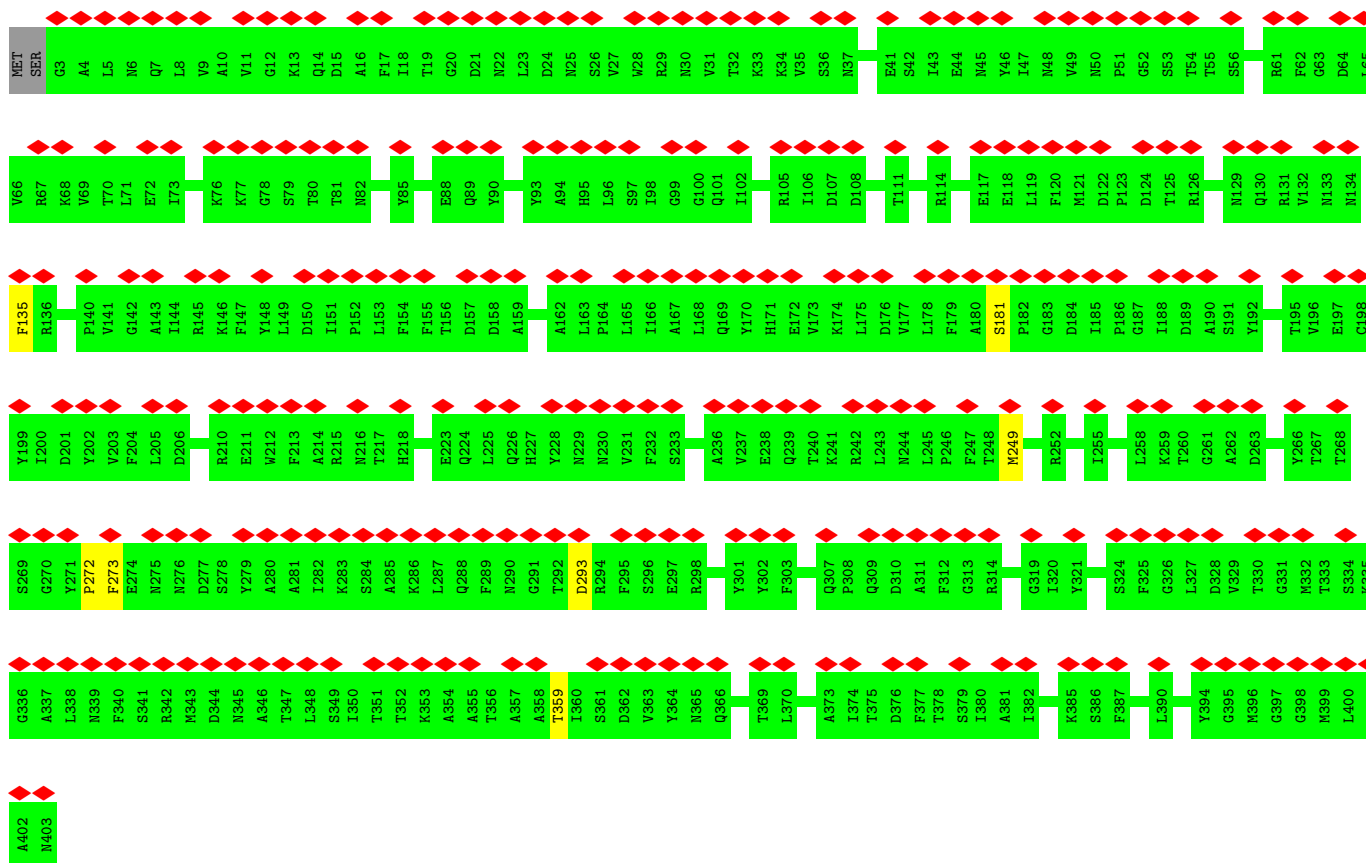
● Molecule 4: MCPv3

Chain bF:

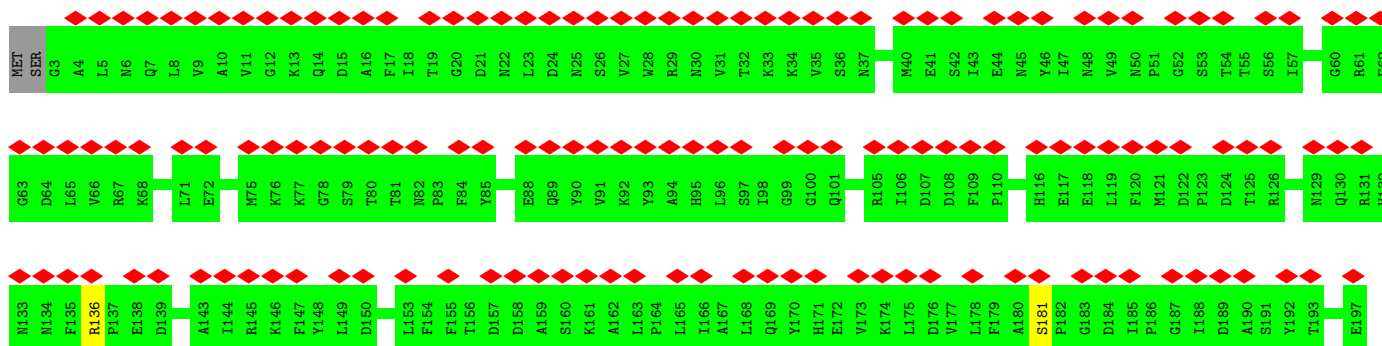


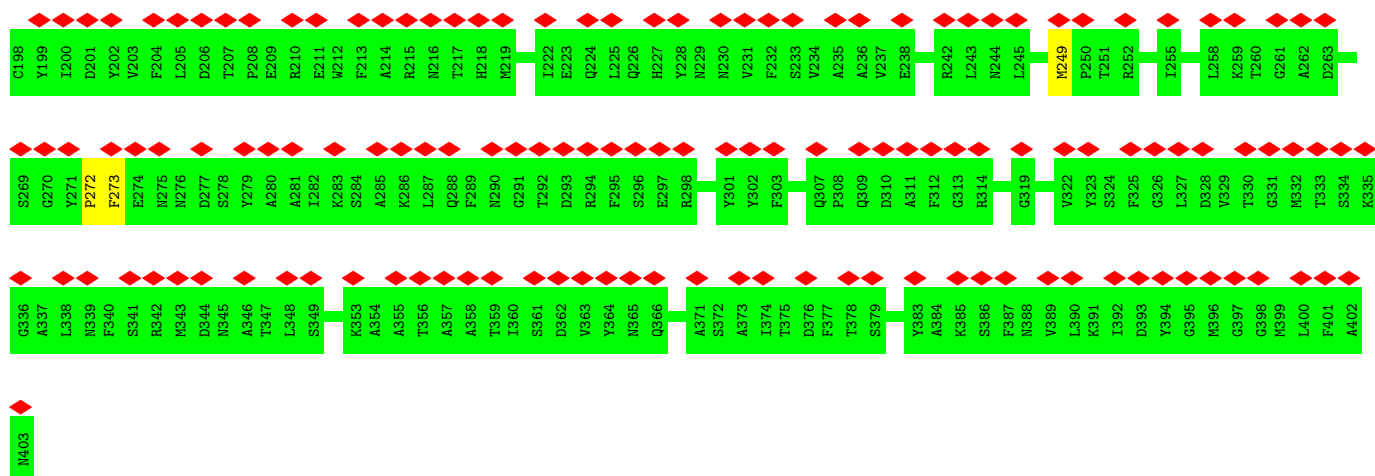


• Molecule 4: MCPv3

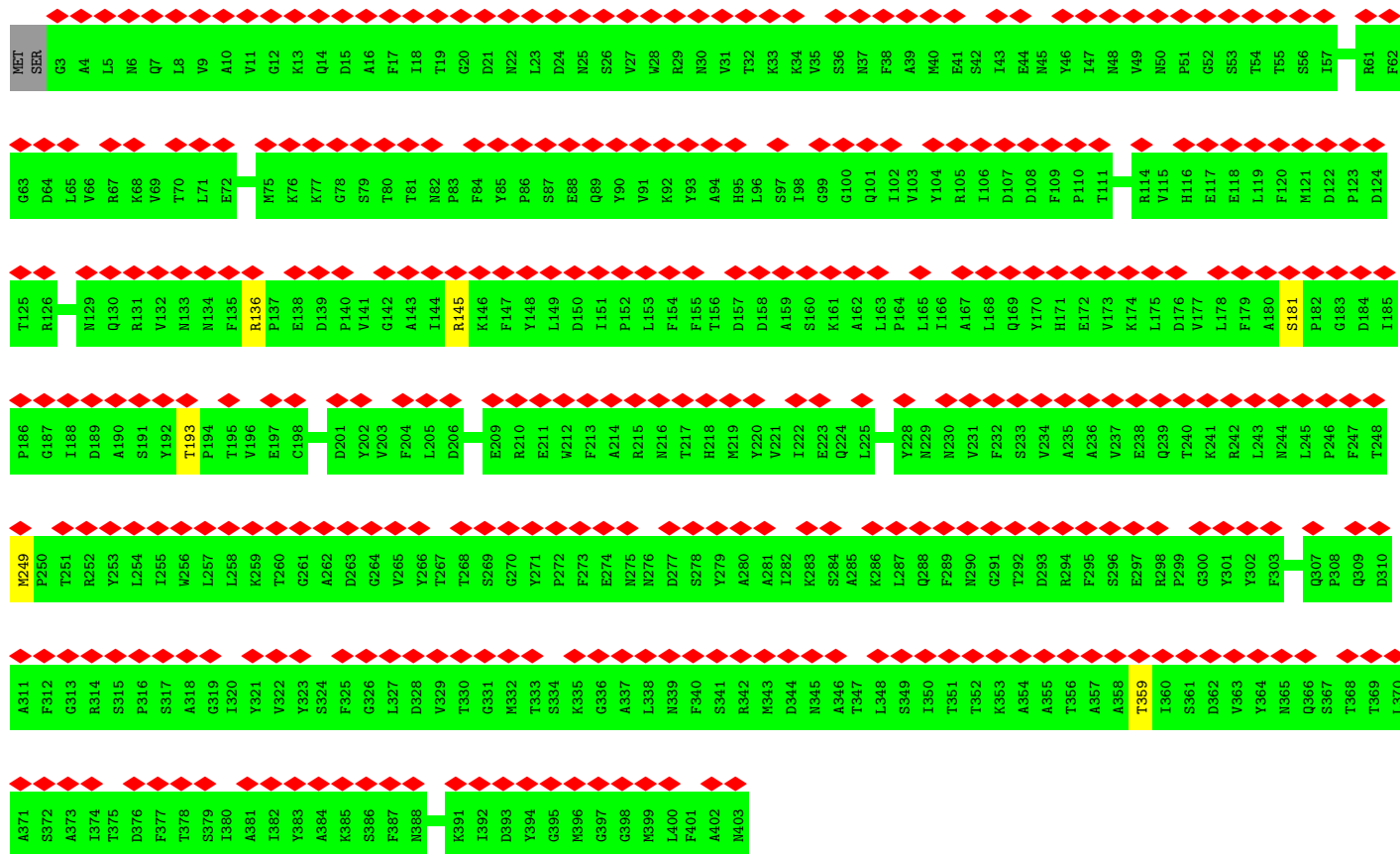
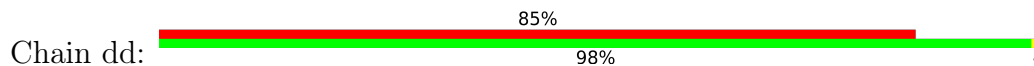


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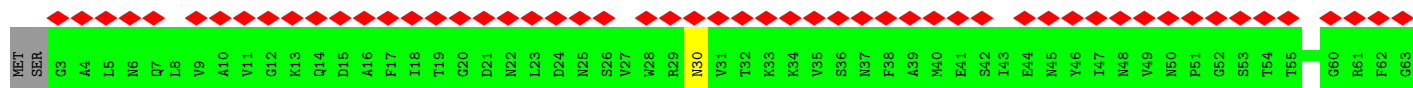
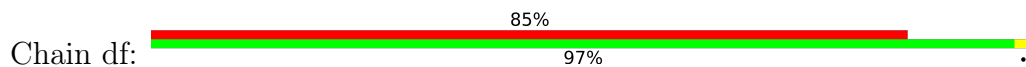




• Molecule 4: MCPv3

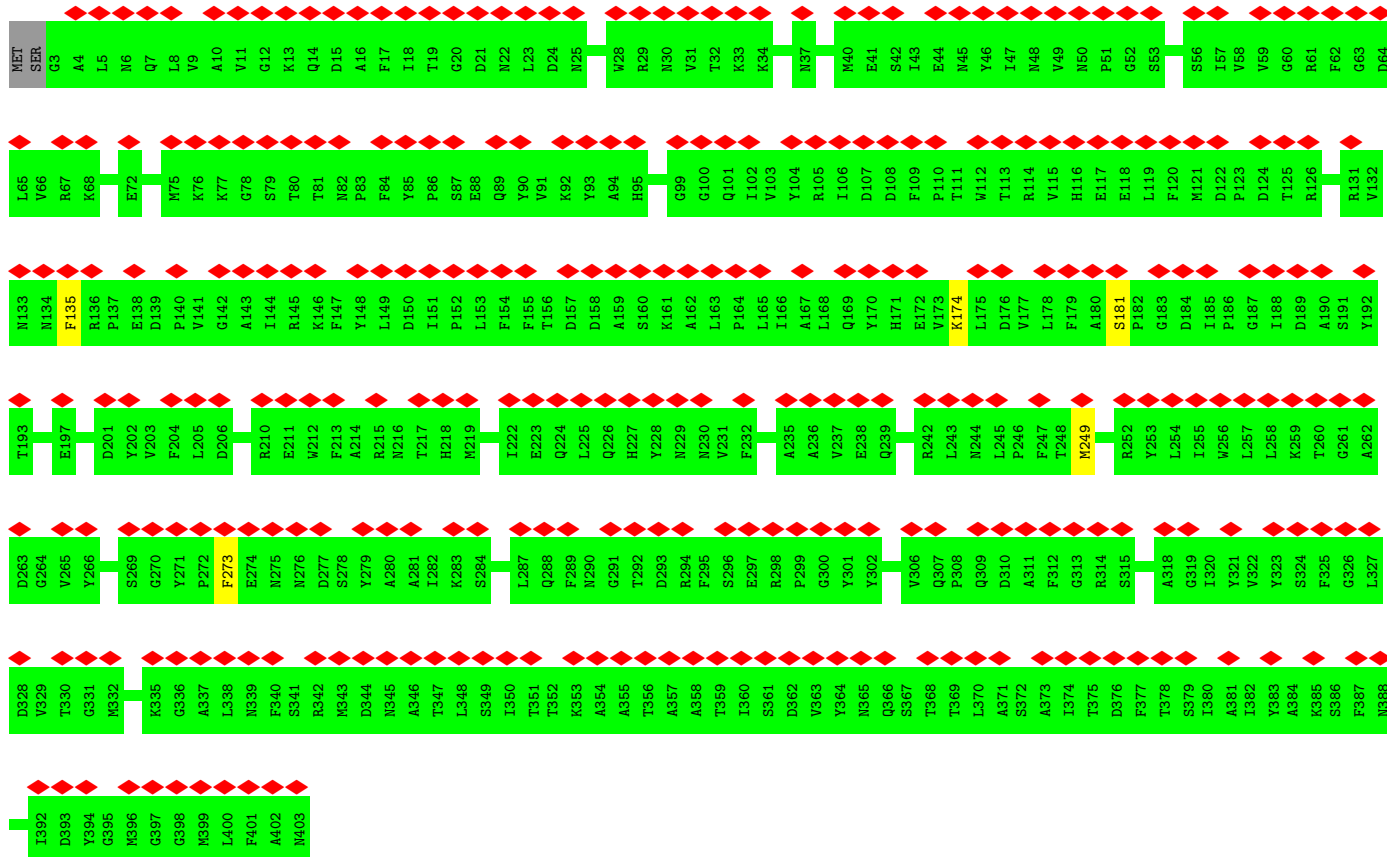
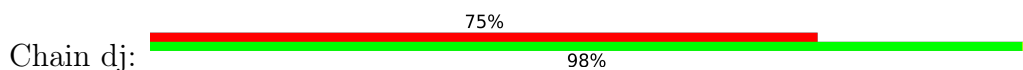


• Molecule 4: MCPv3



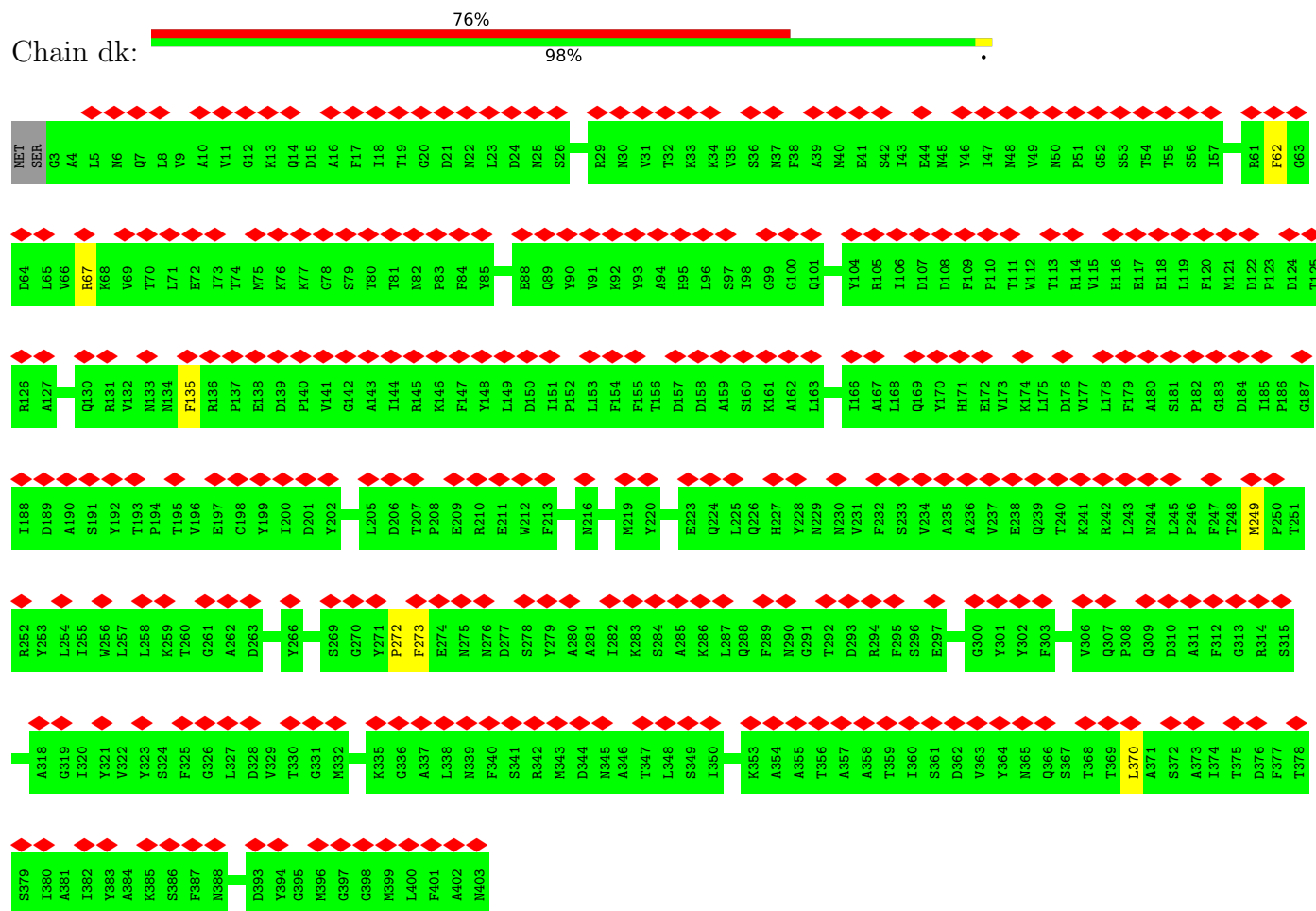


• Molecule 4: MCPv3



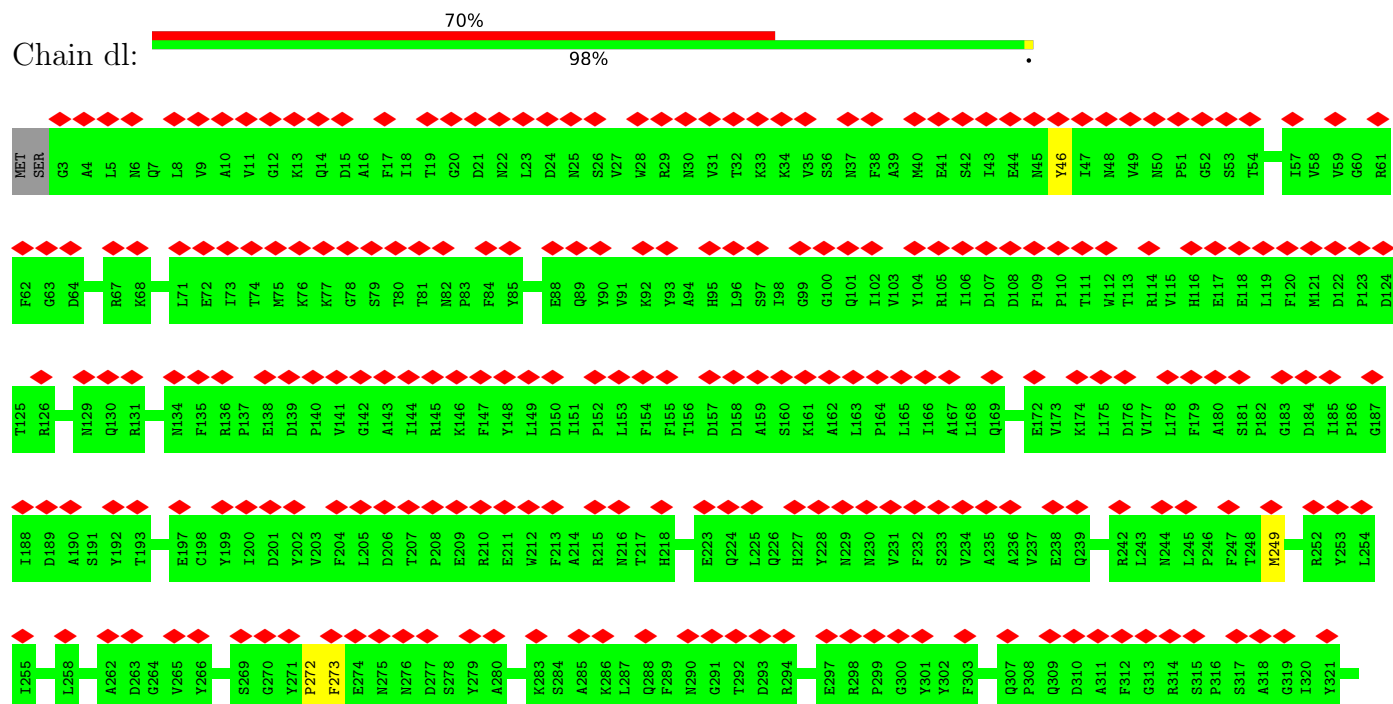
- Molecule 4: MCPv3

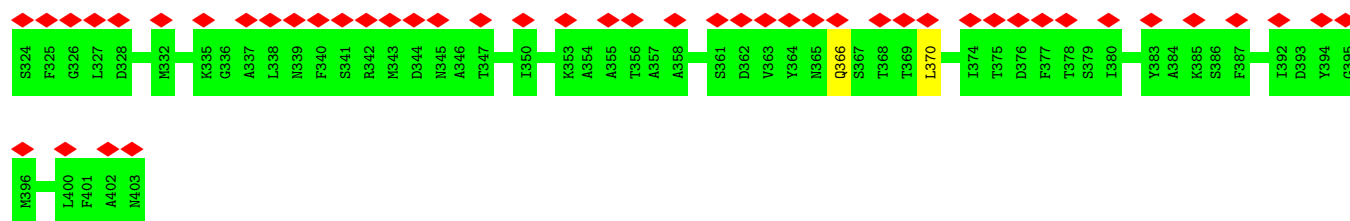
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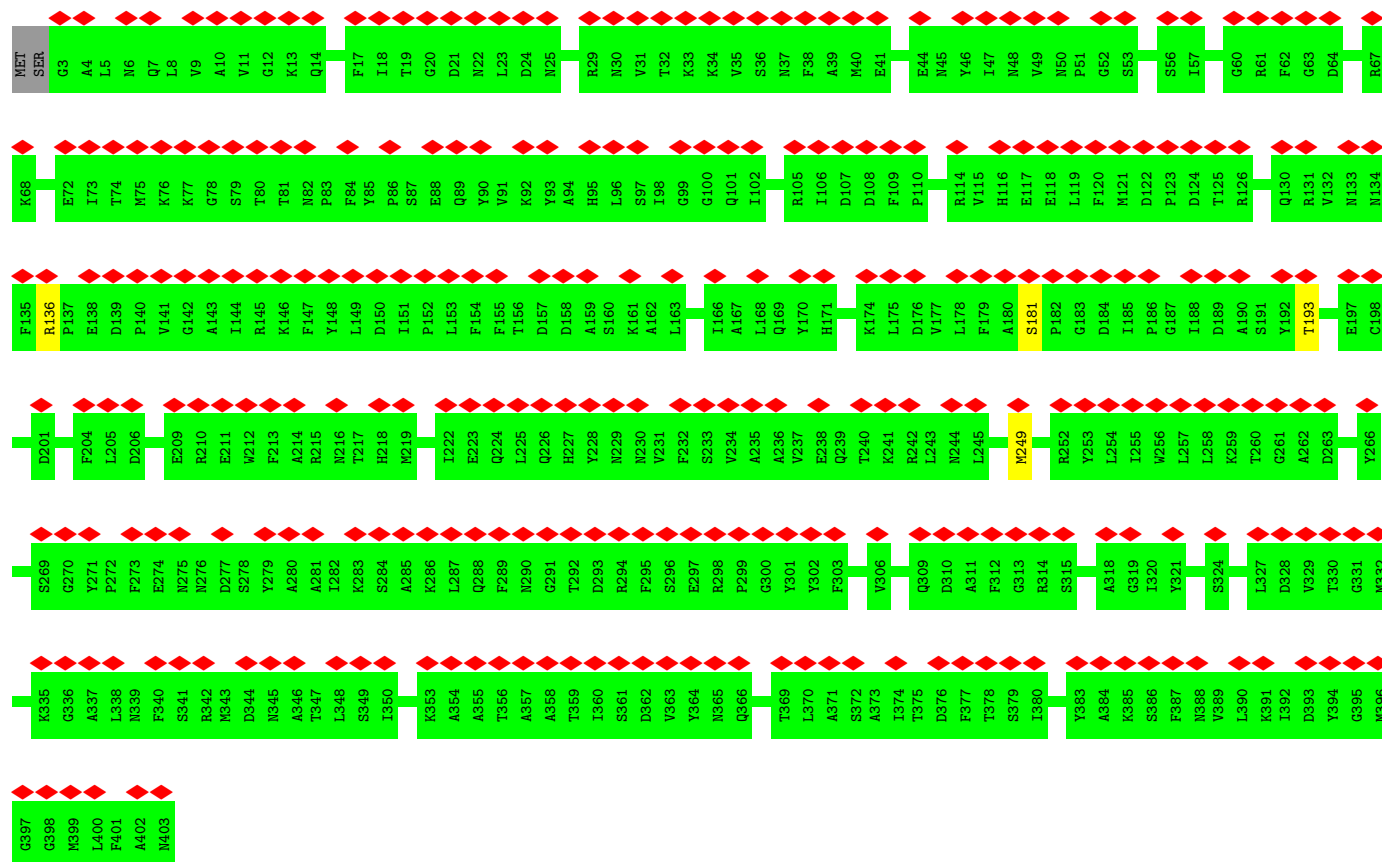
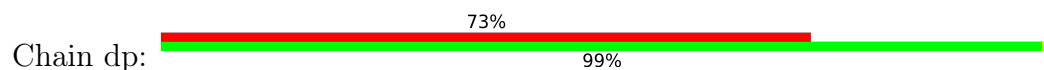
- Molecule 4: MCPv3

Chain dl:

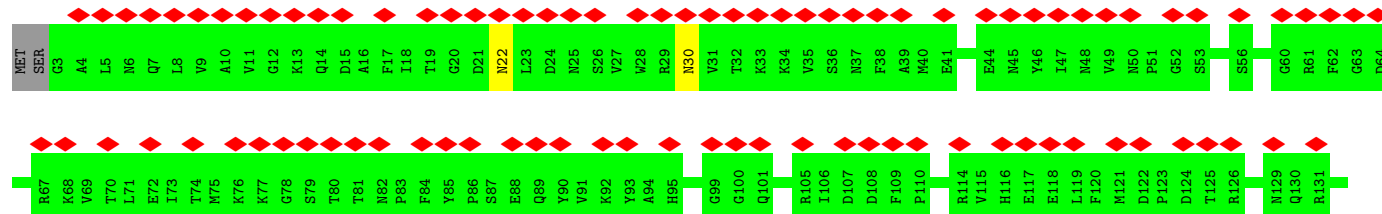


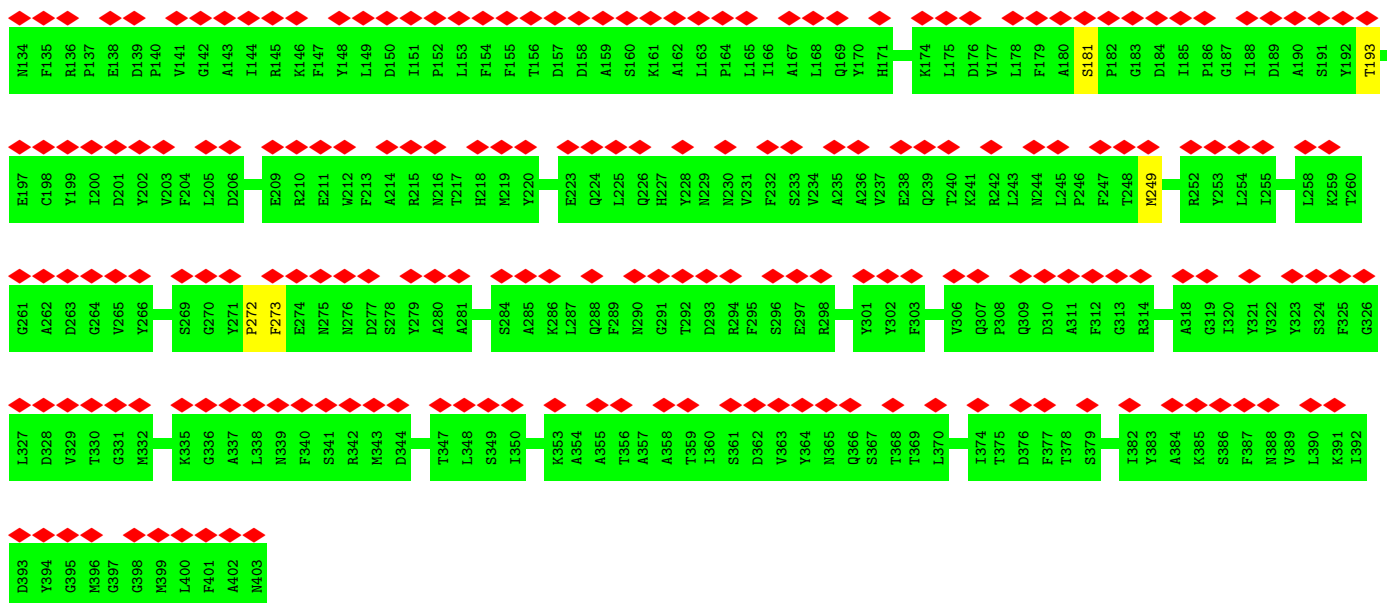


• Molecule 4: MCPv3

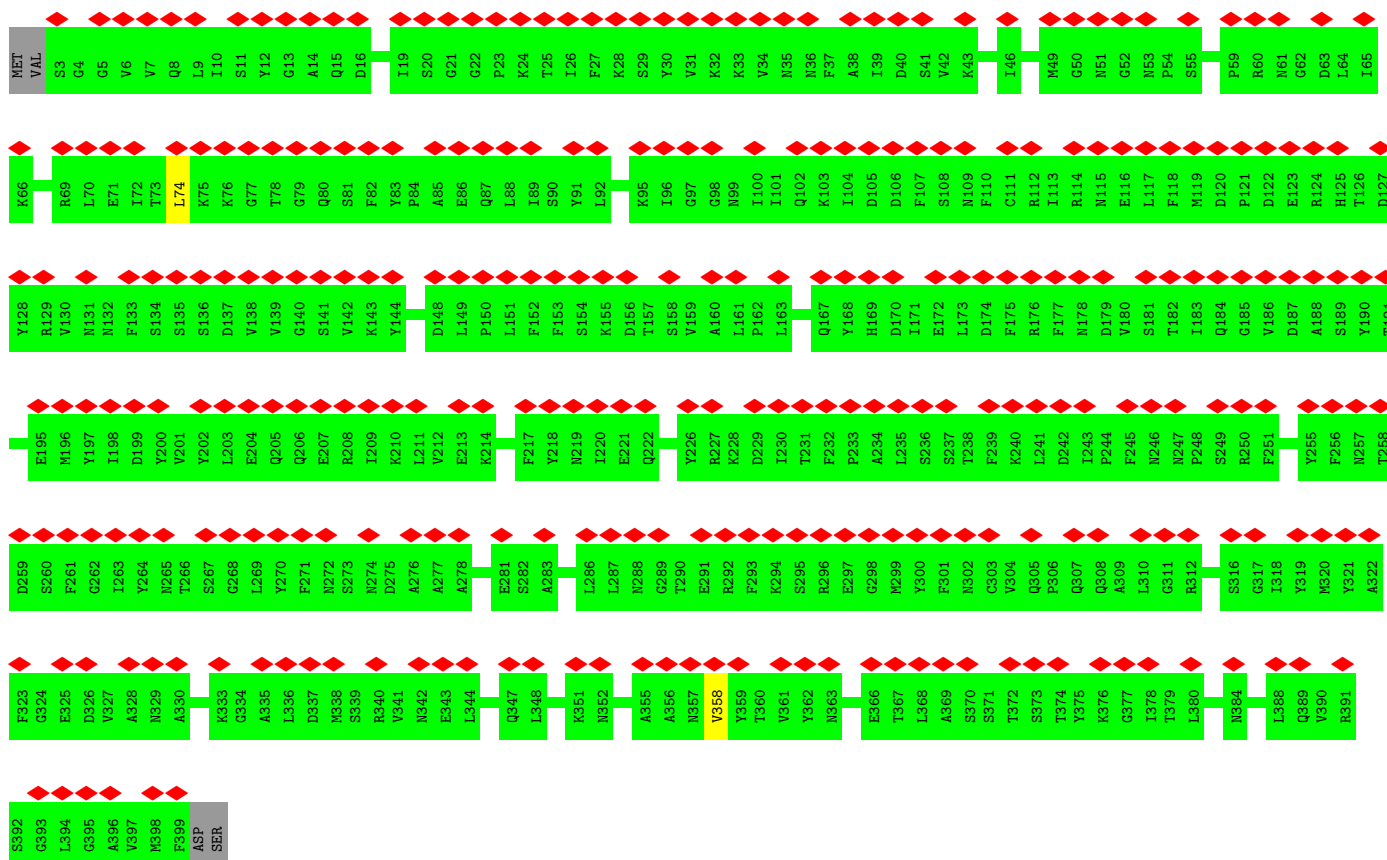
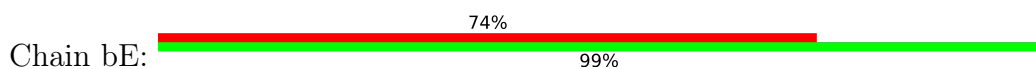


• Molecule 4: MCPv3

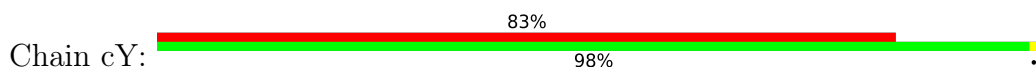


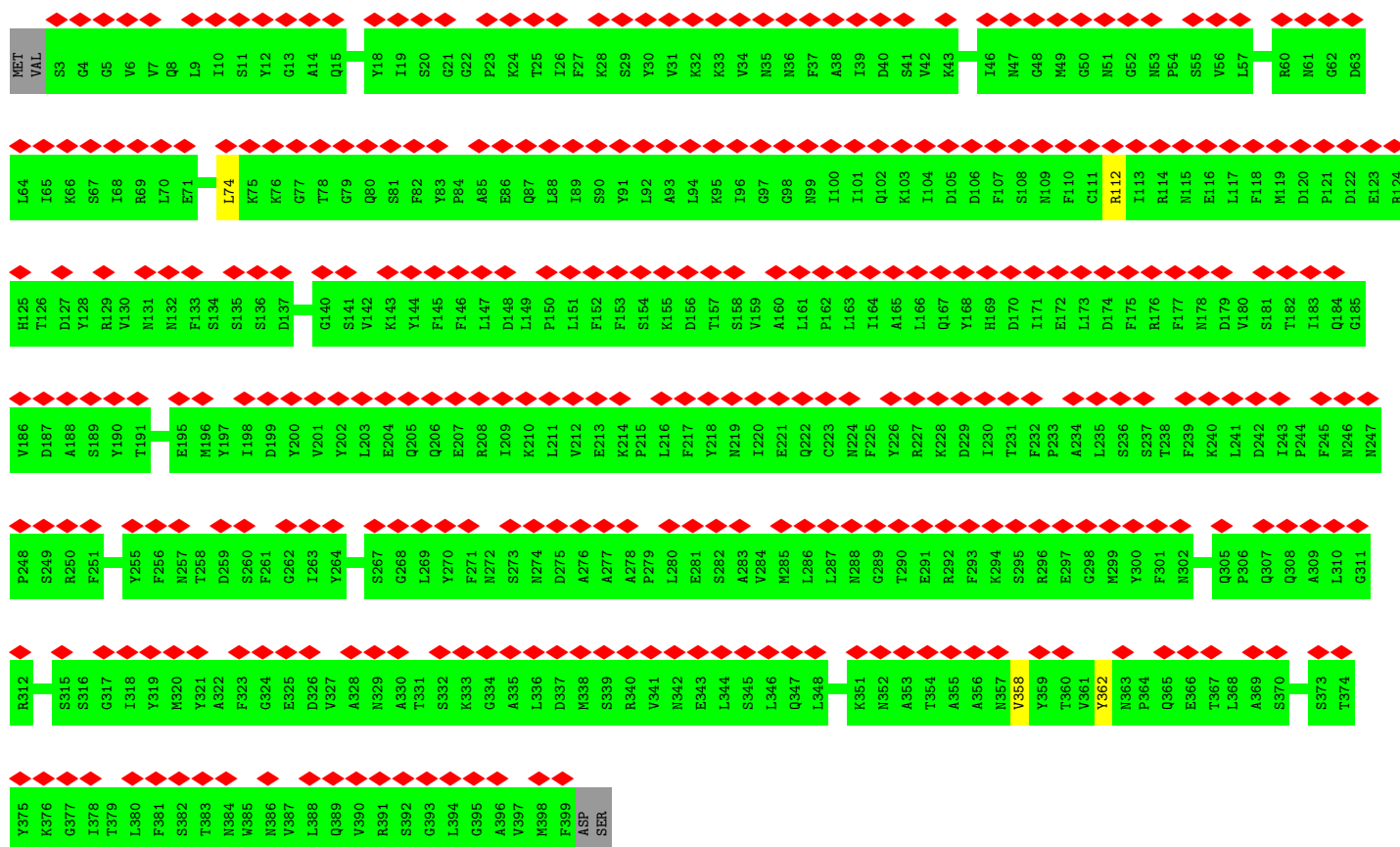


- Molecule 5: MCPv4

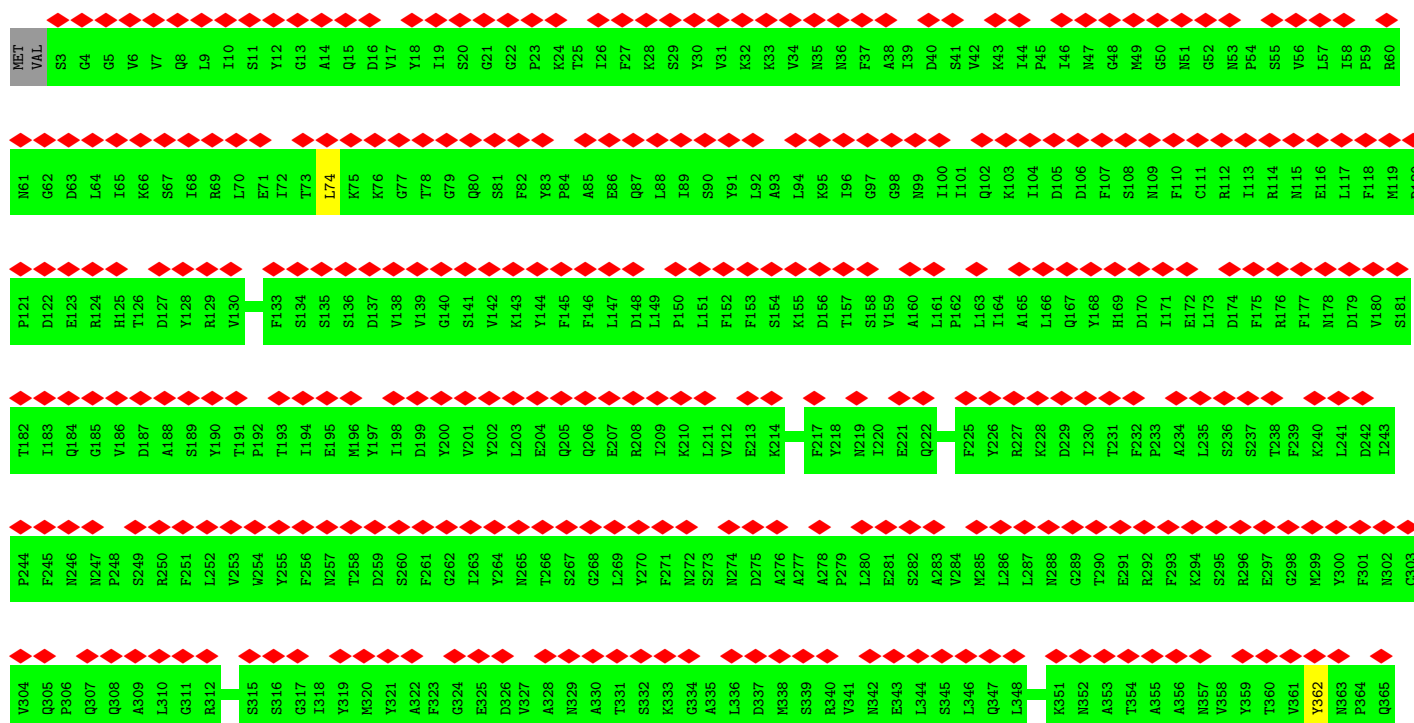
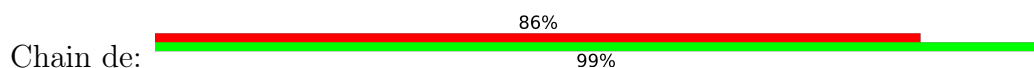


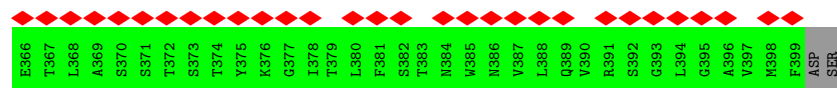
- Molecule 5: MCPv4



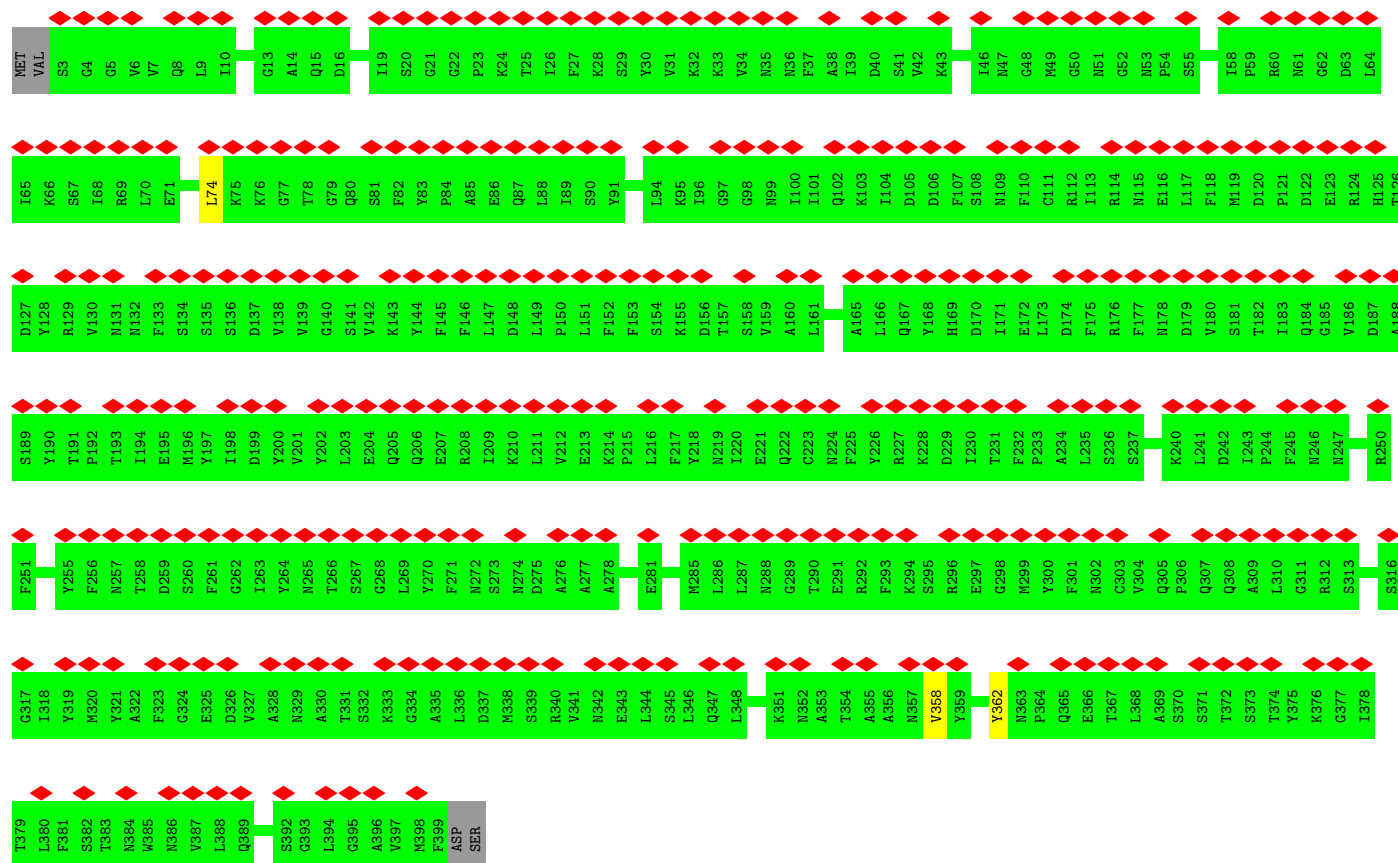
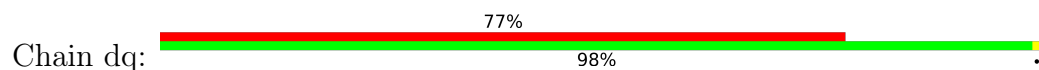


• Molecule 5: MCPv4

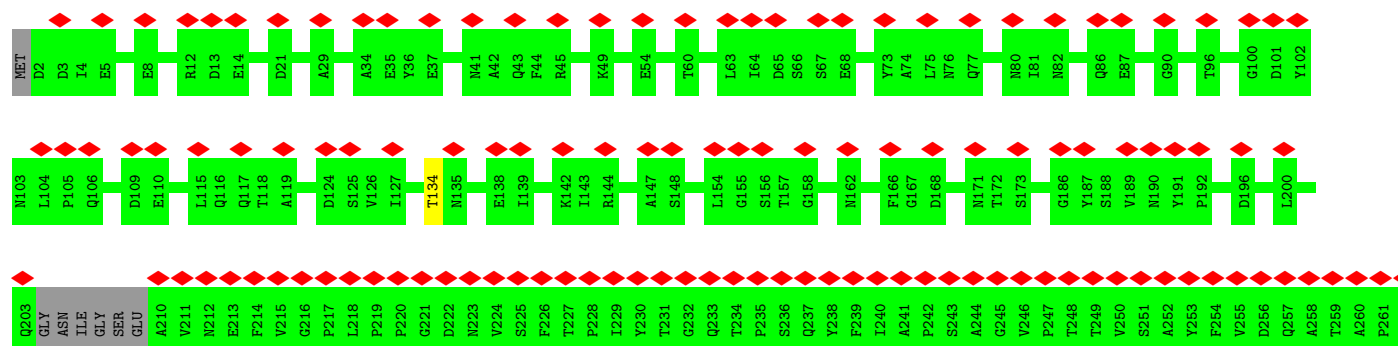




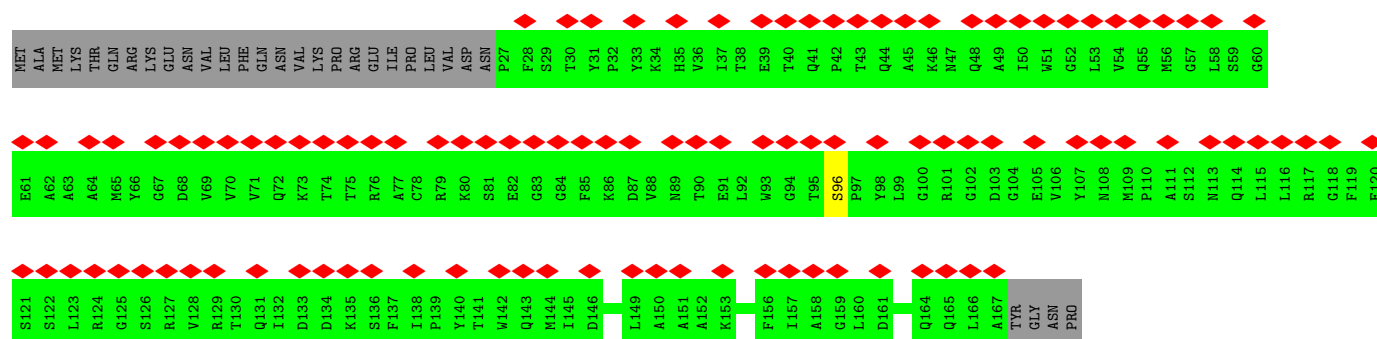
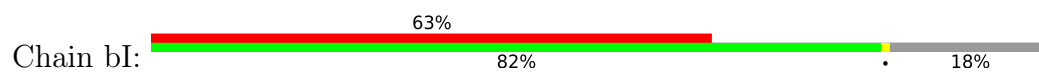
• Molecule 5: MCPv4



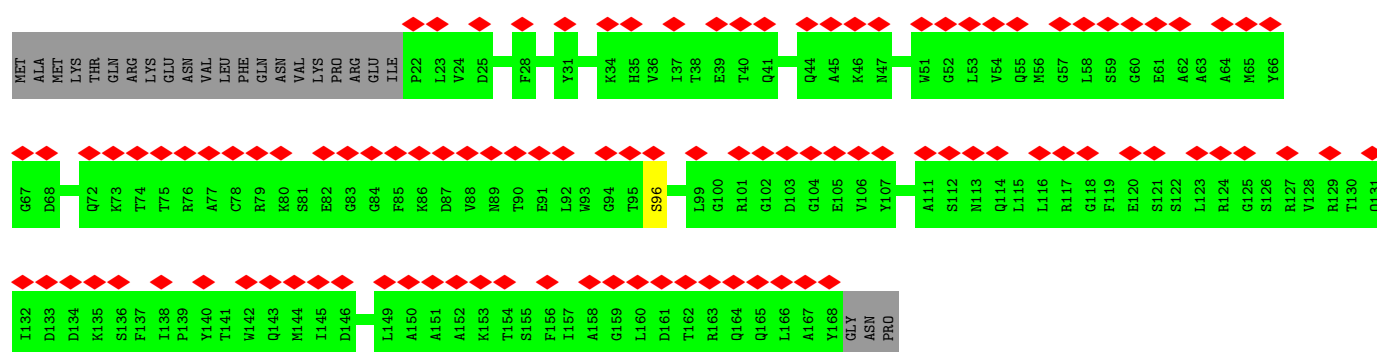
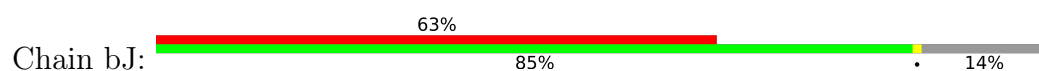
• Molecule 6: P1v1



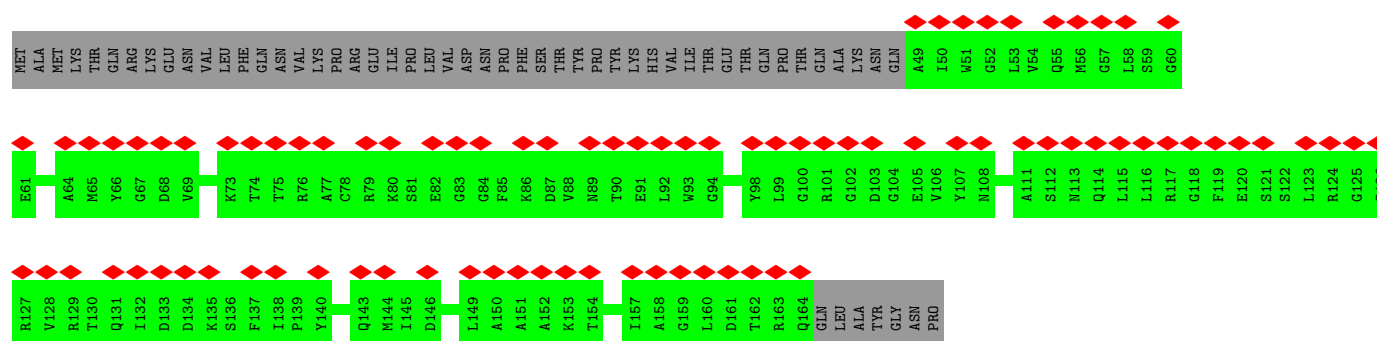




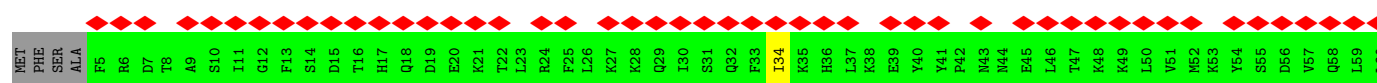
• Molecule 8: P3



• Molecule 8: P3



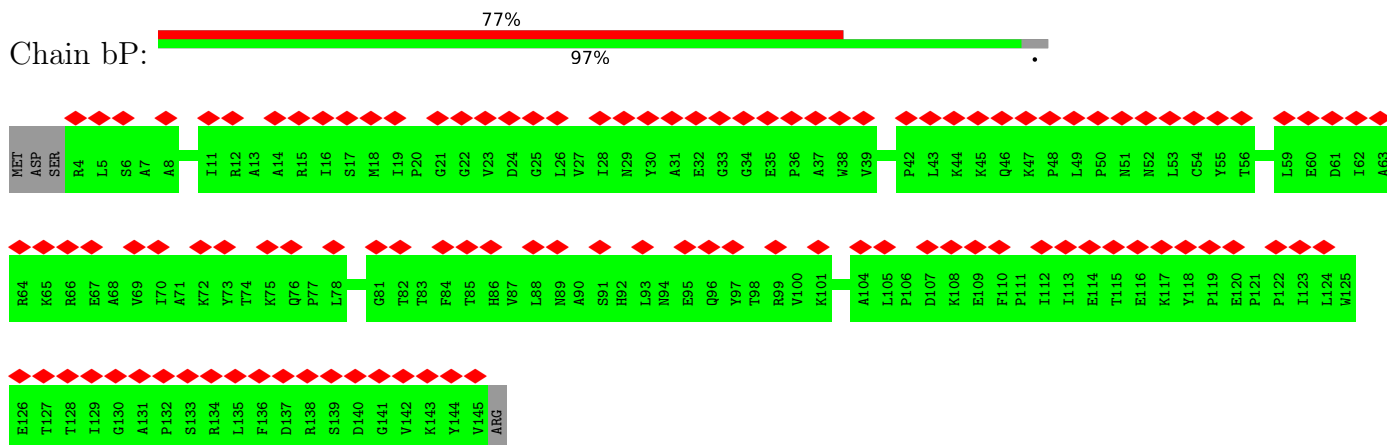
• Molecule 9: P4



ALA

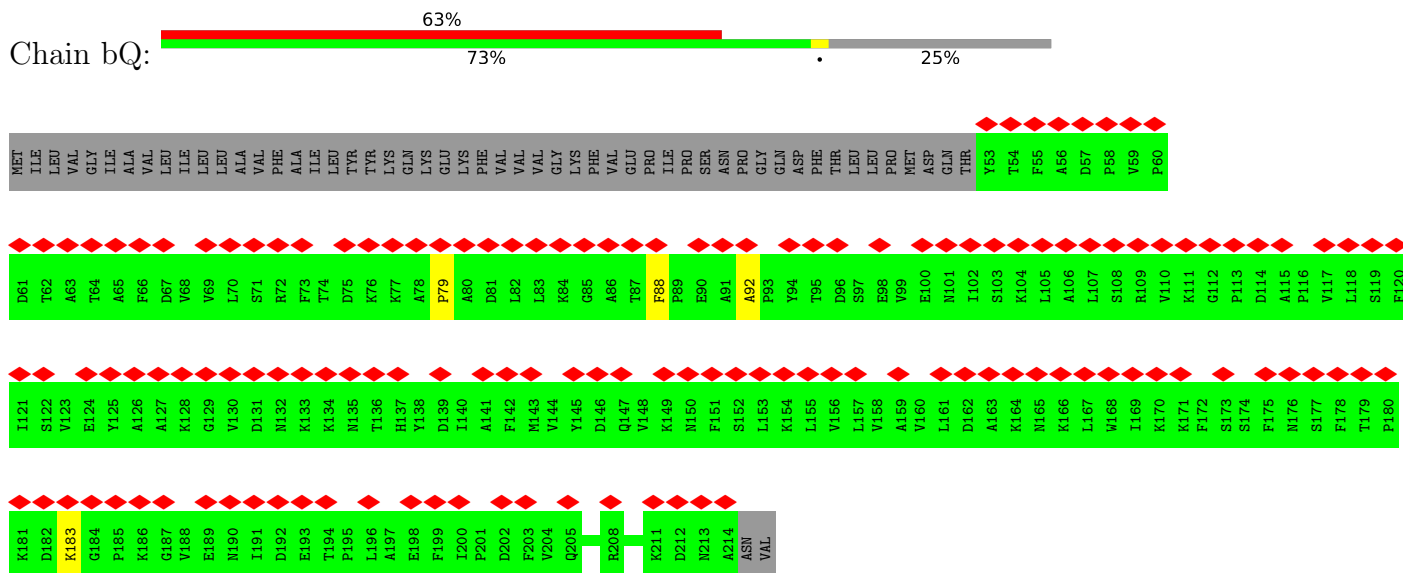
- Molecule 10: P5

Chain bP:



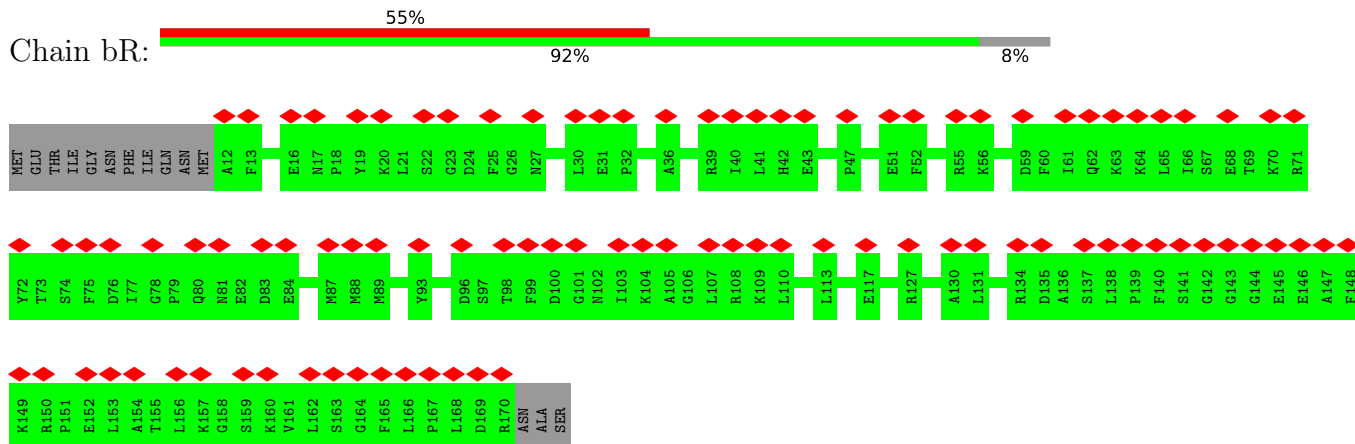
- Molecule 11: P6

Chain bQ:



- Molecule 12: P8

Chain bR:

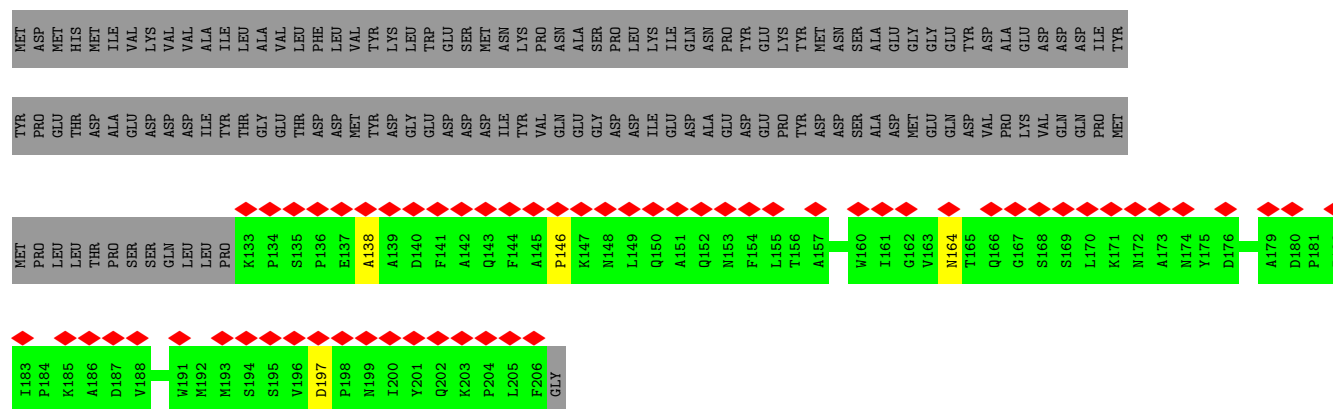


- Molecule 14: P11

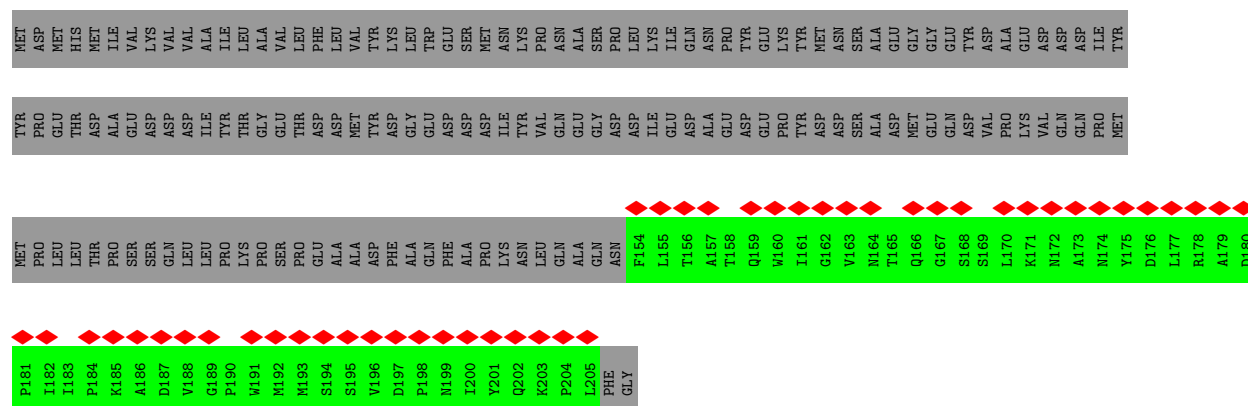
- Molecule 14: P11

- Molecule 14: P11

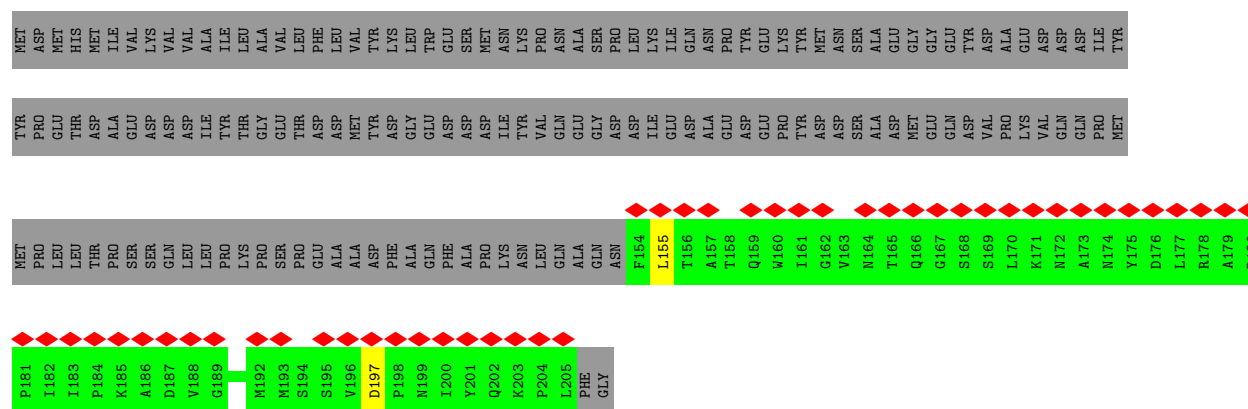




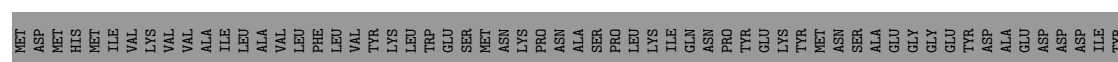
- Molecule 14: P11



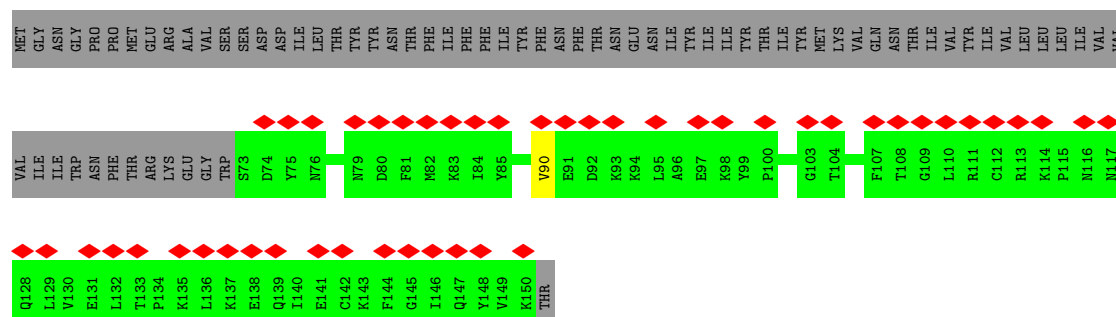
- Molecule 14: P11



- Molecule 14: P11



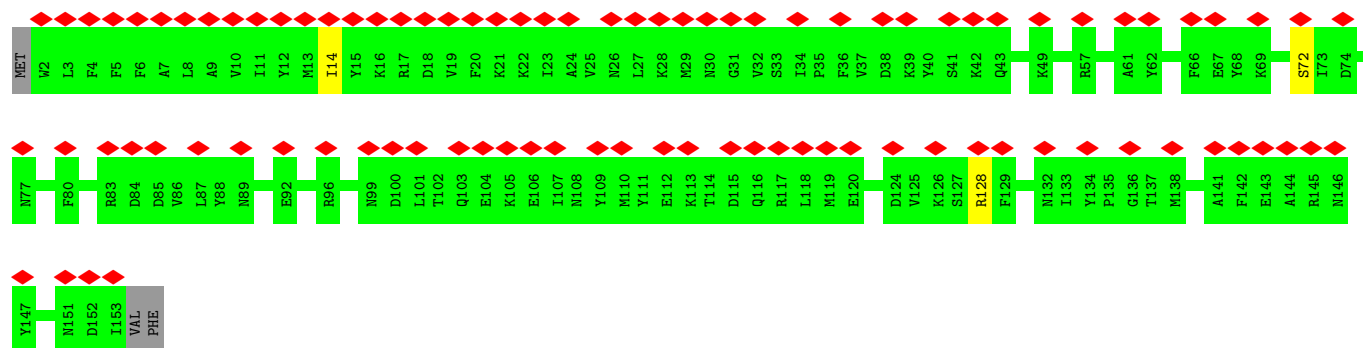
- Molecule 15: P12



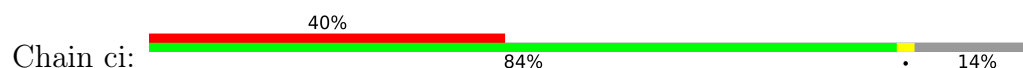
- Molecule 16: P13

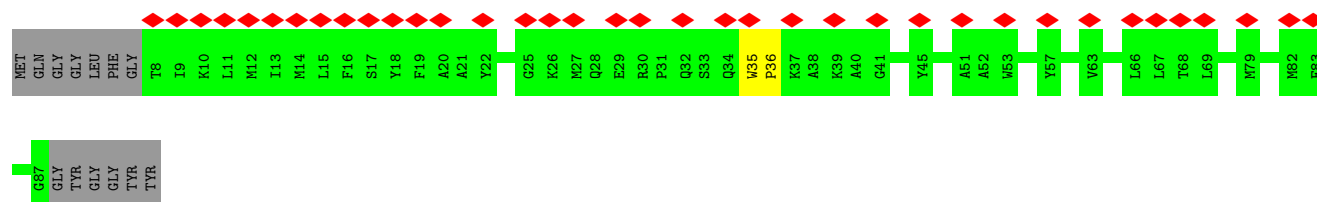


- Molecule 17: P15

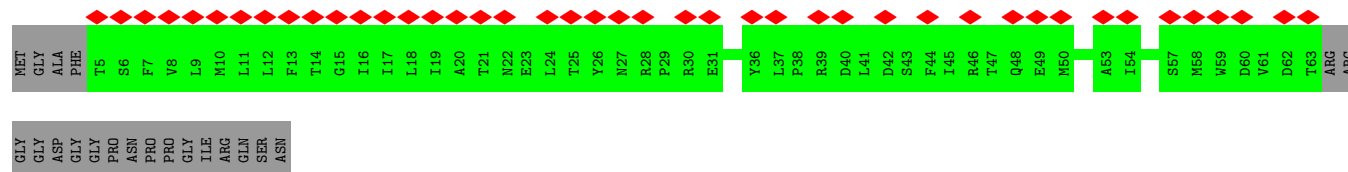
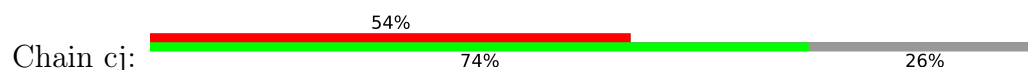


- Molecule 18: P16

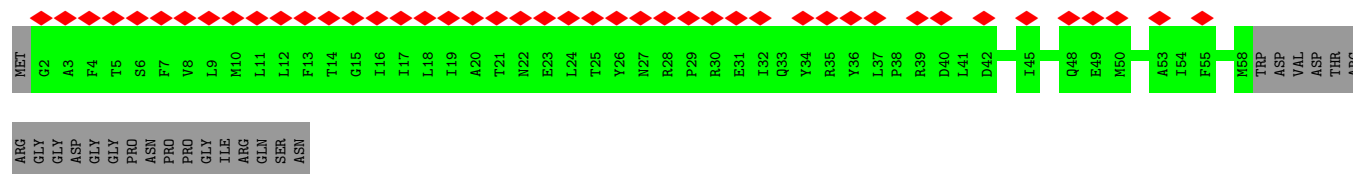
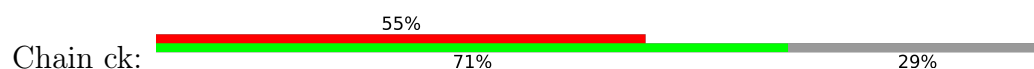




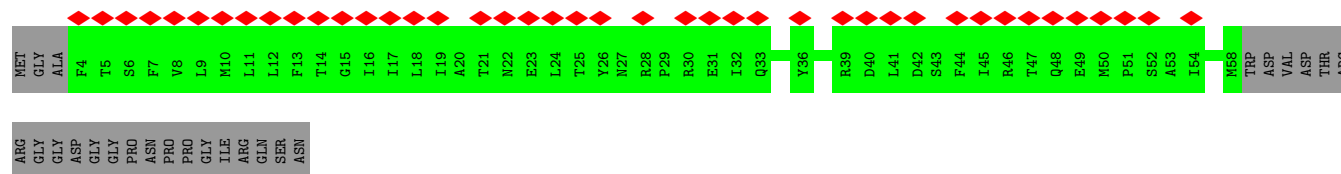
- Molecule 19: P17



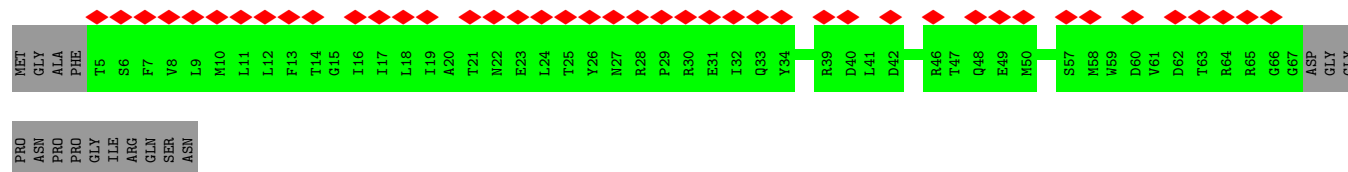
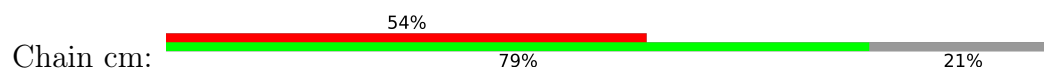
- Molecule 19: P17



- Molecule 19: P17

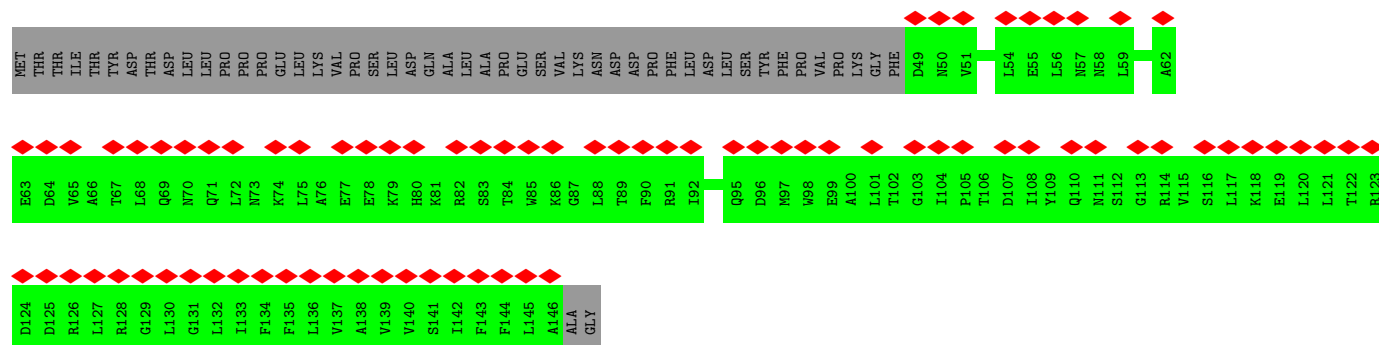


- Molecule 19: P17

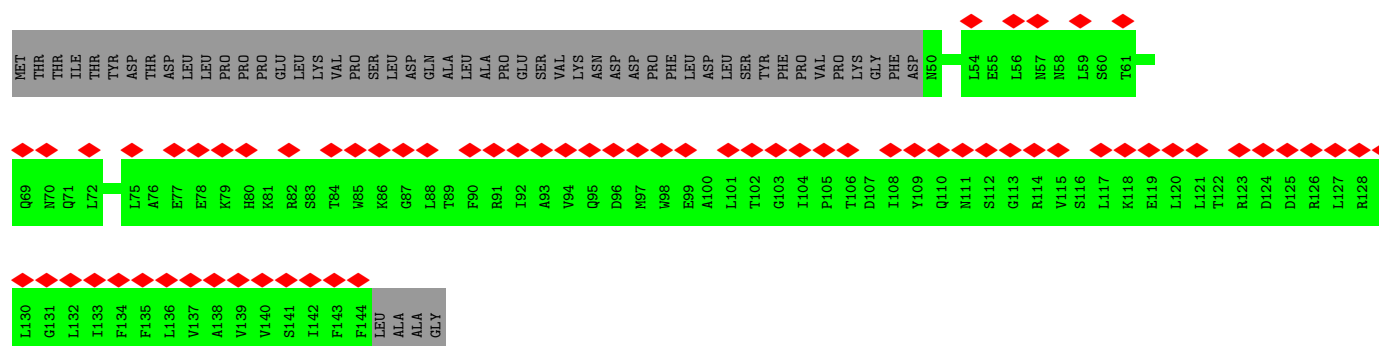


- Molecule 20: P18

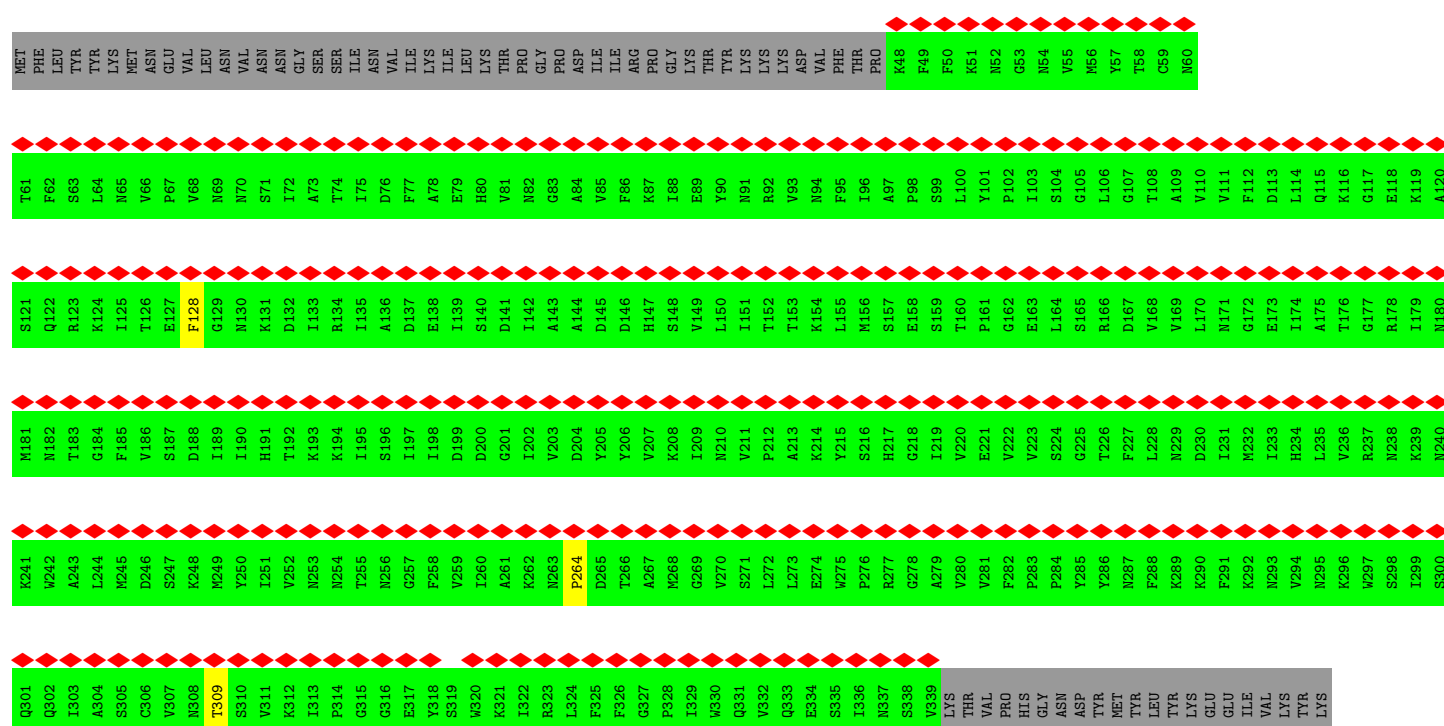
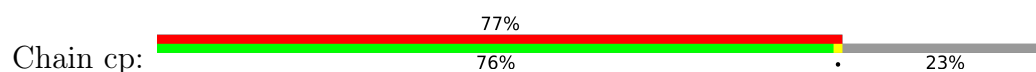




• Molecule 20: P18

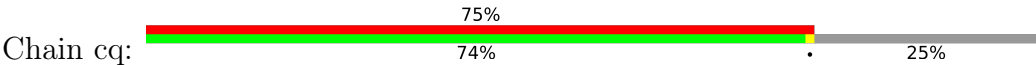


• Molecule 21: P19



TYR	GLN	ARG	ASN	THR	LYS	ARG	ASN	PHE	HIS	GLU	TYR	ASP	TYR	ASP	TYR	LYS	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

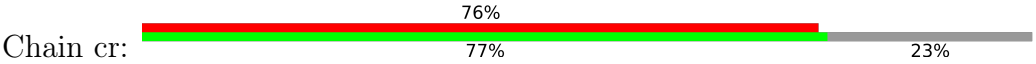
• Molecule 21: P19



MET	PHE	LEU	TTR	LYS	MET	ASN	GLU	VAL	LEU	ASN	VAL	ASN	ASN	GLY	SER	SER	ILE	ASN	VAL	ILE	LYS	LEU	LYS	THR	PRO	PRO	GLY	ASP	ASP	VAL	PHE	THR	PRO	LYS	PHE	PHE	LYS	ASN	GLY	ASN	VAL	MET	TTR	T58	C59	N60																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							

TYR	GLN	ARG	ASN	THR	LYS	ARG	ASN	PHE	HIS	GLU	TYR	ASP	TYR	ASP	TYR	LYS	PHE
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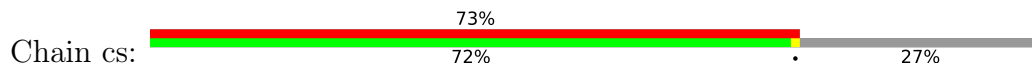
• Molecule 21: P19



MET	PHE	LEU	TYR	TYR	LYS	MET	ASN	GLU	VAL	LEU	ASN	VAL	ASN	ASN	GLY	SER	ILE	ILE	ASN	VAL	ILE	LYS	ILE	LEU	LYS	THR	PRO	GLY	PRO	ASP	ASP	ILE	ILE	ARG	GLY	LYS	THR	TYR	LYS	LYS	ASP	VAL	PHE	THR	PRO	K48	F49	F50	K51	N52	G53	N54	V55	N56	Y57	T58	C59	N60			
T61	F62	S63	L64	N65	V66	P67	V68	N69	N70	S71	I72	A73	T74	I75	D76	F77	A78	E79	H80	I81	N82	G83	A84	N85	F86	A87	K87	I88	E89	Y90	N91	I92	N93	N94	N95	F95	I96	A97	P98	S99	L100	Y101	P102	I103	S104	G105	L106	G107	T108	A109	V110	V111	F112	D113	L114	Q115	K116	G117	E118	K119	A120
S121	Q122	R123	K124	I125	T126	E127	F128	G129	M130	K131	D132	I133	R134	I135	A136	D137	E138	I139	D140	I141	I142	A143	A144	D145	D146	H147	S148	V149	L150	I151	T152	T153	K154	L155	M156	S157	E158	S159	P160	P161	G162	E163	L164	S165	R166	D167	V168	V169	L170	M171	G172	E173	I174	A175	T176	G177	R178	I179	N180		
M181	N182	T183	G184	F185	V186	S187	D188	I189	I190	H191	T192	K193	K194	I195	S196	I197	I198	D199	D200	G201	I202	V203	D204	Y205	Y206	V207	K208	I209	N210	V211	P212	A213	K214	Y215	S216	H217	G218	I219	V220	E221	V222	V223	S224	G225	T226	F227	L228	N229	D230	I231	M232	I233	H234	L235	V236	R237	N238	K239	N240		

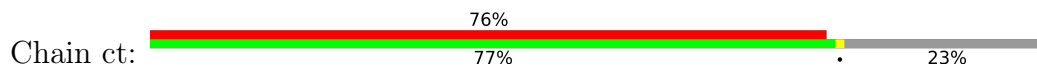
K241	Q301	TYR
W242	Q302	GLN
A243	I303	PHE
L244	A304	LEU
M245	S305	THR
D246	C306	LYS
S247	V307	MET
K248	N308	ASN
M249	T309	HIS
Y250	S310	GLU
I251	V311	VAL
V252	K312	ASN
N253	I313	ASP
N254	S314	TYR
T255	P314	LYS
N256	G315	PHE
G257	G316	
F258	E317	
V259	Y318	
I260	S319	
A261	W320	
K262	K321	
N263	I322	
P264	R323	
D265	L324	
T266	F325	
A267	L326	
M268	G327	
G269	P328	
V270	I329	
S271	W330	
L272	Q331	
L273	V332	
E274	Q333	
W275	E334	
P276	S335	
R277	I336	
G278	N337	
A279	S338	
V280	V339	
V281	LYS	THR
F282	VAL	VAL
P283	PRO	ASN
P284	HIS	VAL
Y285	GLY	GLY
Y286	ASN	ASP
N287	TYR	TYR
F288	MET	MET
K289	LEU	TYR
K290	LYS	LYS
F291	GLU	GLU
K292	ILE	ILE
N293	VAL	VAL
V294	LYS	LYS
N295	TYR	TYR
K296		
W297		
S298		
I299		
S300		

• Molecule 21: P19



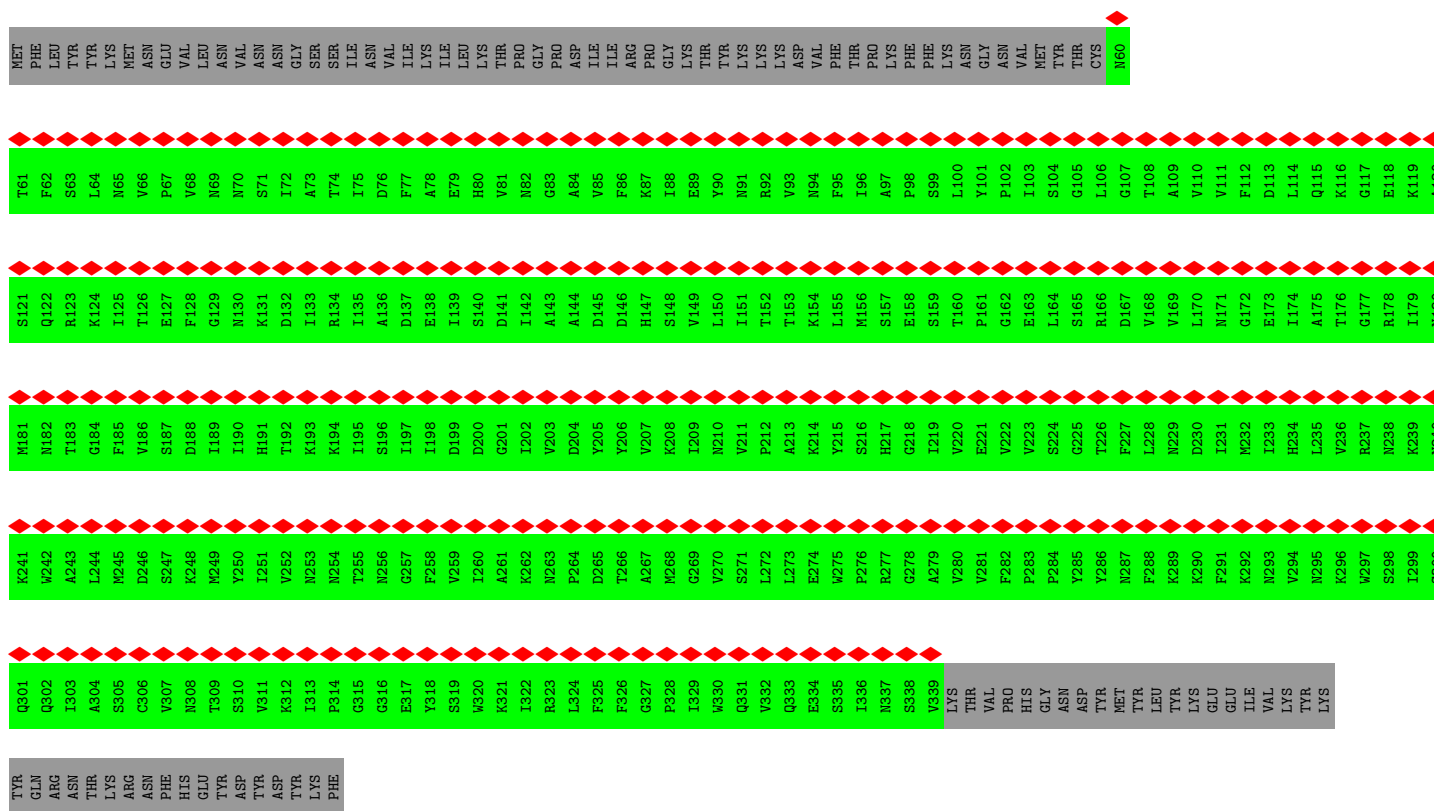
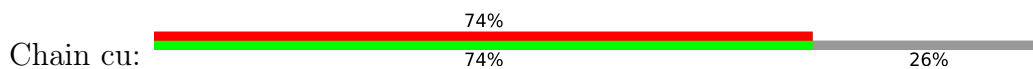
MET	THR	S121	M181	K241	Q301	TYR
PHE	PHE	Q122	N182	W242	Q302	GLN
LEU	LEU	R123	T183	A243	I303	ARG
THR	SER	K124	G184	L244	A304	ASN
LYS	LEU	I125	F185	M245	S305	THR
MET	THR	T126	V186	D246	C306	LYS
ASN	ASN	E127	S187	S247	V307	ARG
PHE	THR	F128	D188	K248	N308	ASN
HIS	LEU	G129	T189	M249	T309	HIS
GLU	VAL	N130	I190	Y250	S310	GLU
VAL	ASN	K131	H191	I251	V311	VAL
ASP	TYR	I132	T192	V252	K312	ASN
TYR	TYR	D133	K193	N253	I313	ASP
PHE	PHE	R134	K194	T254	P314	LYS
		I135	I195	T255	G315	
		A136	S196	N256	G316	
		D137	I197	G257	E317	
		E138	I198	F258	Y318	
		I139	D199	V259	W320	
		S140	D200	I260	K321	
		D141	G201	A261	I322	
		I142	T202	K262	R323	
		A143	V203	N263	L324	
		A144	D204	P264	F325	
		D145	Y205	D265	L326	
		D146	Y206	T266	G327	
		H147	V207	A267	P328	
		S148	K208	M268	I329	
		V149	I209	G269	W330	
		I150	N210	V270	Q331	
		I151	V211	S271	V332	
		T152	P212	L272	Q333	
		T153	A213	L273	E334	
		K154	K214	E274	S335	
		L155	Y215	W275	I336	
		M156	S216	P276	N337	
		S157	H217	R277	S338	
		E158	G218	G278	V339	
		S159	I219	A279	LYS	THR
		T160	V220	V280	VAL	VAL
		P161	E221	V281	PRO	ASN
		G162	V222	F282	HIS	VAL
		E163	V223	P283	GLY	GLY
		L164	S224	P284	ASN	ASP
		S165	G225	Y285	TYR	TYR
		R166	T226	V286	MET	MET
		D167	F227	N287	LEU	TYR
		V168	L228	F288	LYS	LYS
		V169	N229	K289	GLU	GLU
		L170	D230	K290	ILE	ILE
		N171	I231	F291	VAL	VAL
		G172	M232	K292	LYS	LYS
		T173	I233	N293	TYR	TYR
		I174	H234	V294		
		A175	L235	N295		
		T176	V236	K296		
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		E178	R238	S298		
		I179	K239	I299		
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• Molecule 21: P19

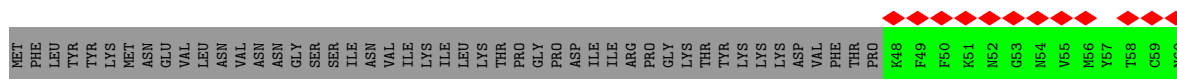
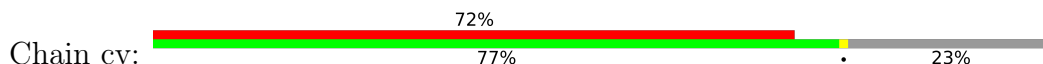


MET	T61	S121
PHE	F62	Q122
LEU	S63	R123
TYR	L64	K124
LYS	N65	I125
MET	V66	T126
ASN	P67	E127
VAL	F68	F128
LEU	N69	G129
ASN	N70	M130
VAL	S71	K131
ASN	T72	D132
GLY	A73	I133
SER	T74	R134
ILE	I75	I135
ASN	D76	A136
VAL	F77	D137
ILE	E78	E138
LYS	H80	I139
LEU	V81	S140
LYS	I82	D141
THR	G83	A143
PRO	A84	A144
GLY	F85	D145
ASP	H86	D146
ILE	K87	H147
ILE	I88	S148
ARG	E89	V149
GLY	Y90	L150
LYS	N91	I151
THR	R92	T152
LYS	V93	T153
ASP	N94	K154
VAL	P95	L155
PHE	I96	M156
THR	A97	S157
PRO	K48	E158
	F49	S159
	F50	P160
	K51	P161
	N52	G162
	G53	E163
	N54	L164
	V55	S165
	M56	R166
	Y57	D167
	F58	V168
	C59	V169
		L170
		N171
		G172
		E173
		I174
		A175
		T176
		G177
		E178
		I179
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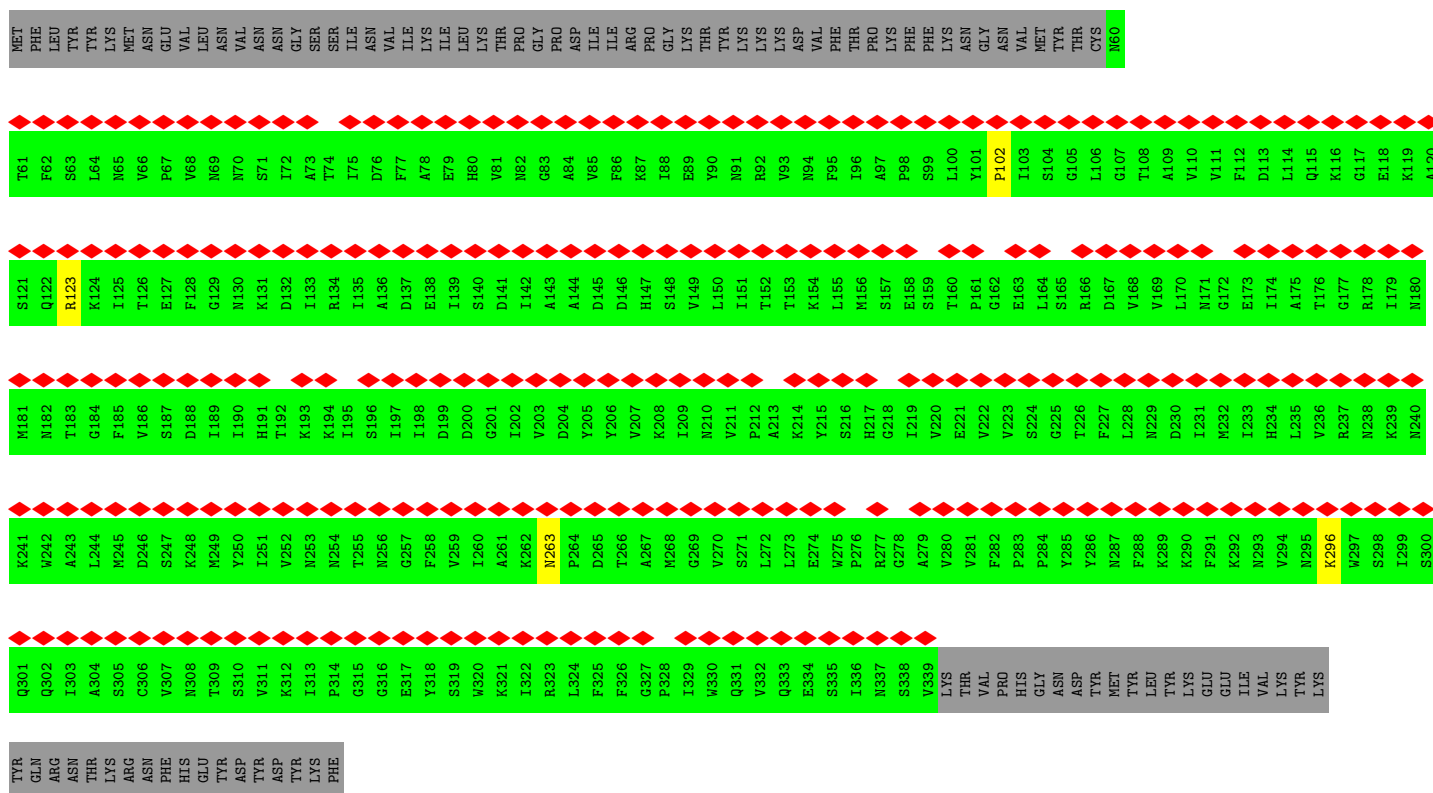
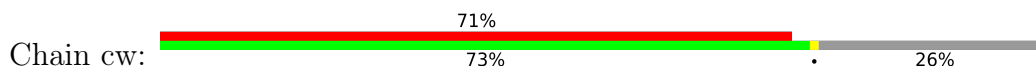
- Molecule 21: P19



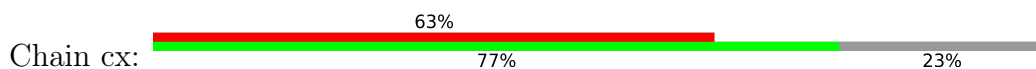
- Molecule 21: P19



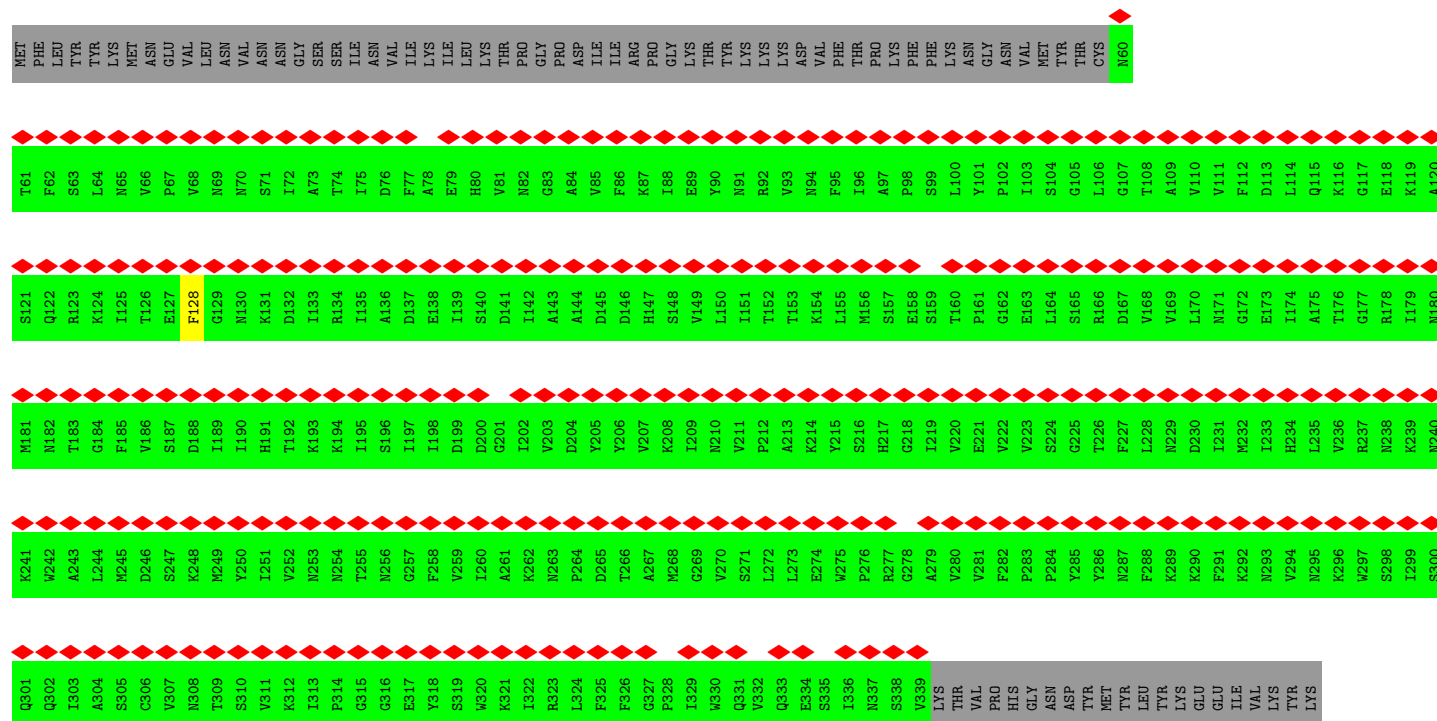
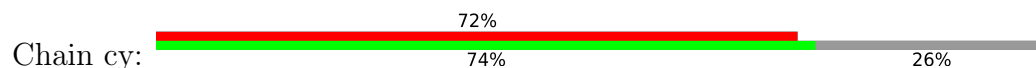
- Molecule 21: P19

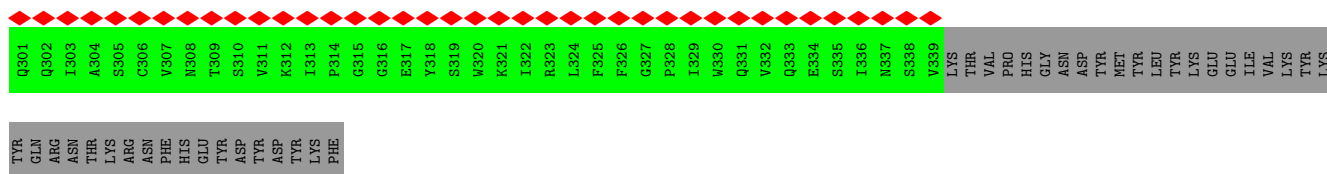


- Molecule 21: P19

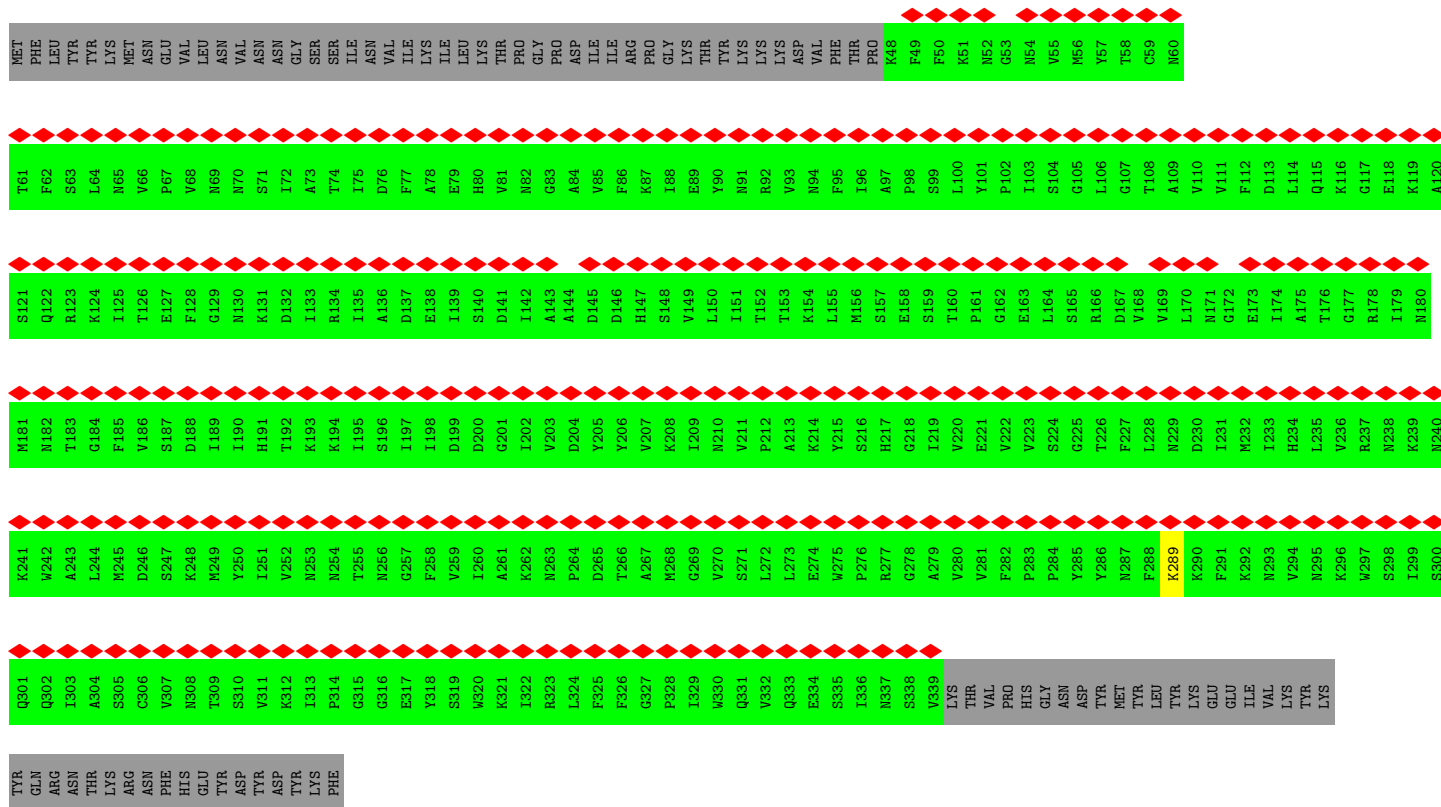
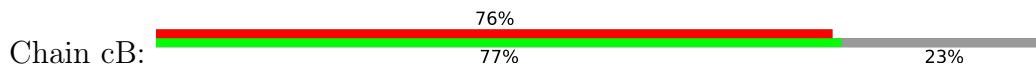


- Molecule 21: P19

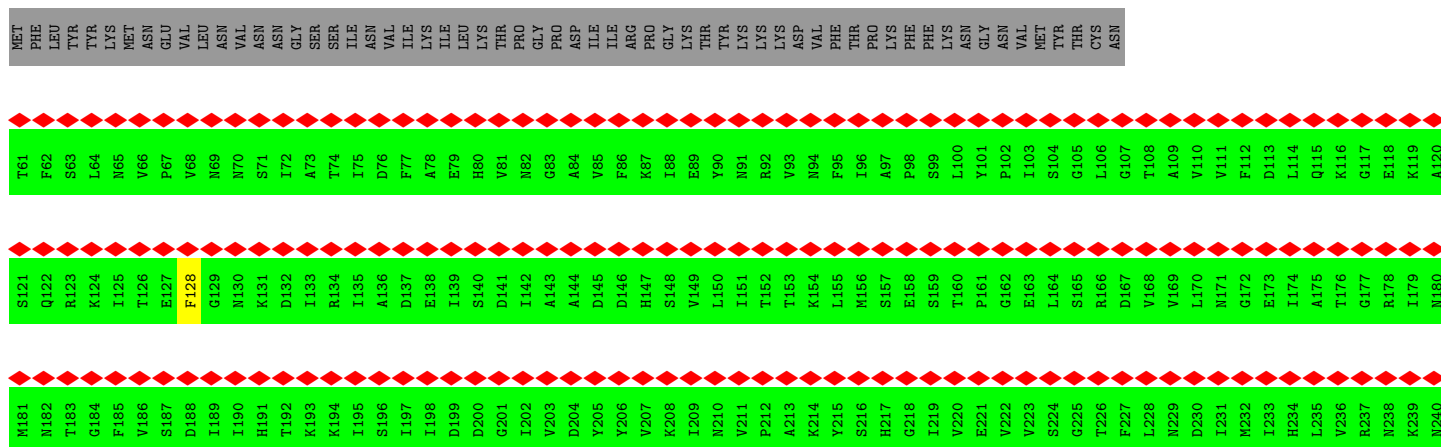
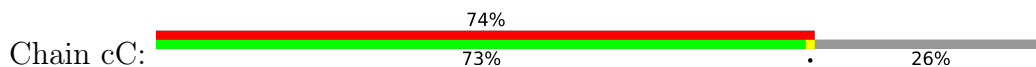




• Molecule 21: P19

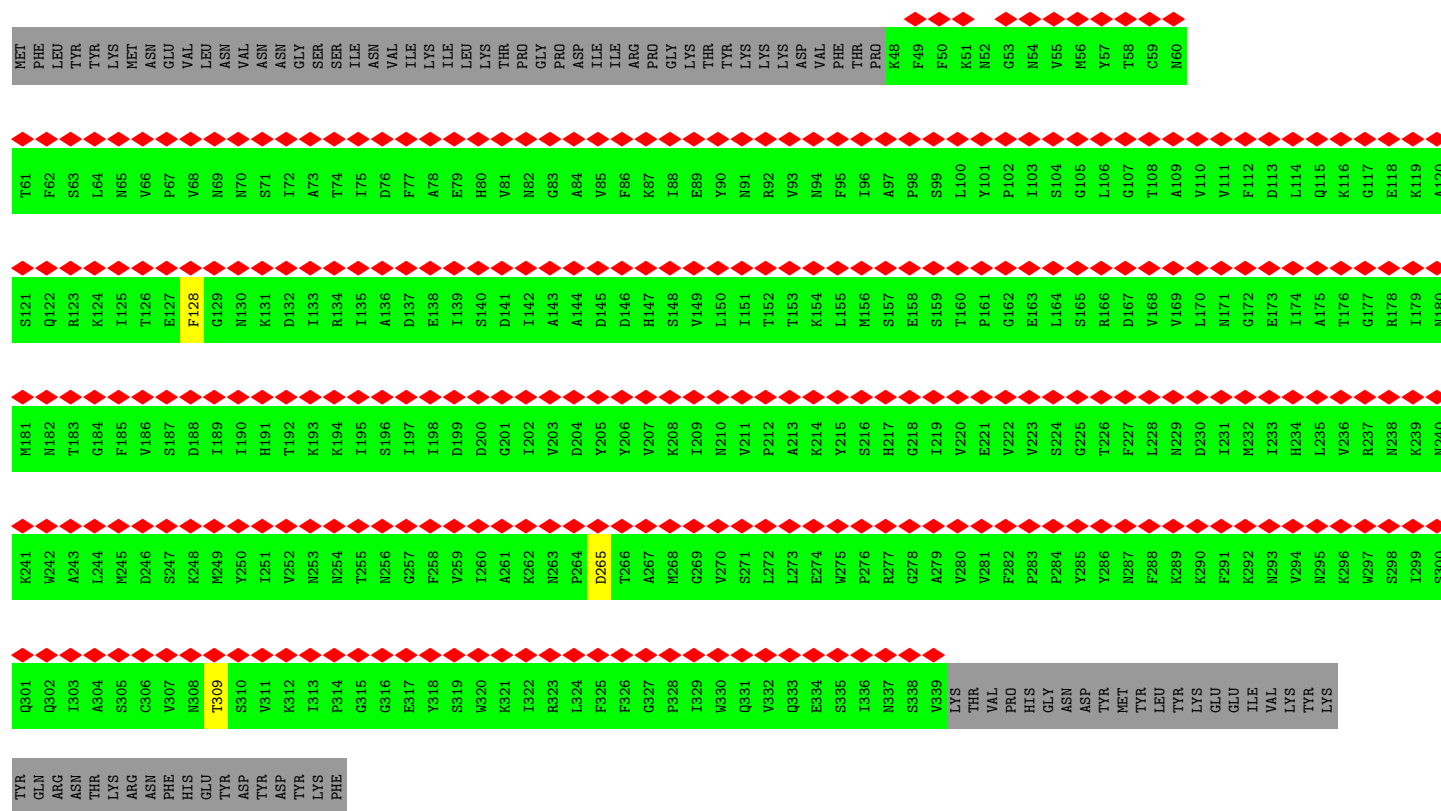
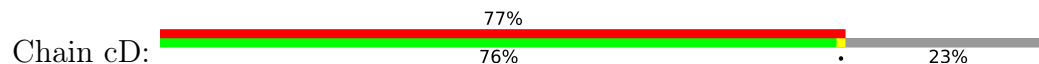


• Molecule 21: P19

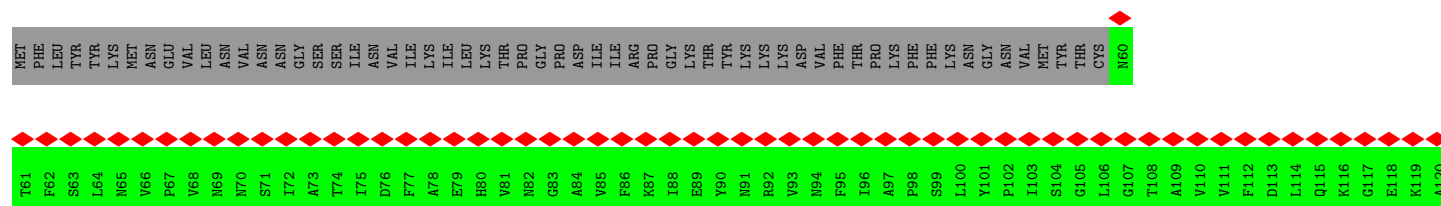




• Molecule 21: P19

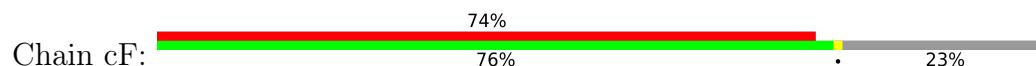


• Molecule 21: P19



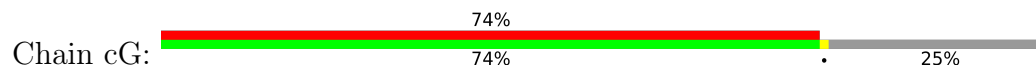
S121	M181	K241	Q301	TYR
Q122	N182	W242	Q302	GLN
R123	T183	W243	I303	ARG
K124	G184	A243	I304	ASN
I125	F185	L244	A304	THR
T126	V186	M245	S305	LYS
E127	S187	D246	C306	ARG
F128	D188	S247	PHE	ASN
G129	I189	K248	N308	HIS
M130	I190	M249	T309	GLU
K131	H191	Y250	S310	TYR
D132	T192	I251	V311	TYR
I133	T193	V252	K312	ASP
R134	K194	N253	I313	LYS
I135	I195	N254	P314	LYS
A136	S196	T255	G315	PHE
D137	S197	N256	G316	
E138	I198	G257	Y318	
I139	D199	F258	S319	
S140	D200	V259	W320	
D141	G201	I260	K321	
I142	I202	A261	I322	
A143	V203	K262	R523	
A144	D204	N263	L324	
D145	Y205	D264	F325	
D146	Y206	T265	F326	
H147	V207	T266	G327	
S148	K208	A267	P328	
V149	I209	M268	I329	
L150	N210	G269	W330	
I151	V211	V270	Q331	
T152	P212	S271	V332	
T153	A213	L272	Q333	
K154	K214	L273	E334	
L155	Y215	E274	S335	
M156	S216	W275	I336	
S157	H217	P276	N337	
E158	G218	G277	S338	
S159	I219	A279	V339	
T160	E221	V280	THR	
P161	V222	V281	VAL	
E163	V223	F282	PRO	
L164	S224	P283	HIS	
S165	G225	P284	GLY	
R166	G226	Y285	ASN	
D167	T226	Y286	TYR	
V168	F227	N287	TYR	
V169	L228	F288	LEU	
L170	N229	K289	TYR	
M171	D230	K290	LYS	
G172	I231	F291	GLU	
E173	M232	K292	ILE	
I174	I233	N293	VAL	
A175	H234	V294	LYS	
T176	L235	N295	LYS	
G177	V236	K296		
R178	R237	W297		
I179	K239	S298		
N180		I299		
		S300		

• Molecule 21: P19




RET	T61	S121	M182	W242	Q302	ARG
PHE	F62	Q122	T183	A243	I303	ASN
LEU	S63	R123	G184	M245	A304	THR
TYR	L64	K124	F185	D246	S305	LYS
LYS	N65	I125	V186	S247	C306	PHE
MET	V66	T126	S187	K248	HIS	GLU
ASN	P67	E127	D188	M249	TYR	ASP
VAL	V68	F128	I189	Y250	TYR	PHE
ASN	N69	G129	I190	I251	V311	
ASN	N70	M130	H191	V252	K312	
ASN	S71	K131	T192	N253	I313	
GLY	I72	D132	K193	M254	P314	
SER	A73	I133	K194	T255	G315	
ILE	T74	R134	I195	N256	E317	
ASN	I75	I135	S196	G257	Y318	
VAL	D76	A136	I197	F258	S319	
ILE	F77	D137	I198	V259	W320	
LYS	A78	E138	D199	I260	K321	
LEU	E79	I139	D200	A261	I322	
LYS	H80	S140	G201	K262	R523	
THR	W81	D141	I202	F264	L324	
PRO	N82	I142	V203	T265	F325	
GLY	G83	A143	D204	T266	F326	
ASP	A84	A144	Y205	H147	I329	
ILE	W85	D145	Y206	S148	Q331	
ILE	F86	D146	V207	V149	V332	
ARG	K87	H147	K208	L150	Q333	
PRO	R88	S148	I209	I151	E334	
GLY	E89	V149	N210	T152	K154	
LYS	Y90	L150	V211	T153	L155	
THR	N91	I151	P212	K154	S216	
LYS	R92	T152	A213	L155	H217	
ASP	V93	T153	K214	S216	G218	
VAL	N94	K154	W275	M156	I219	
PHE	F95	L155	P276	S157	V220	
THR	I96	M156	R277	E158	E221	
PRO	A97	S157	G278	T160	V222	
K48	P98	G218	A279	P161	V223	
F49	S99	I219	V280	E162	G224	
F50	L100	V220	V281	E163	S224	
K51	Y101	E221	F282	L164	Y285	
N52	P102	V222	P283	S165	T226	
O53	I103	V223	P284	R166	F227	
N54	S104	G225	Y285	D167	L228	
V55	G105	T226	MET	V168	K289	
M56	L106	F227	TYR	N229	D230	
V57	G107	L228	LEU	D230	I231	
T58	T108	V168	TYR	I231	M232	
C59	A109	V169	LYS	M232	I233	
N60	V110	L170	VAL	I233	H234	
	V111	E173	LYS	H234	L235	
	F112	I174	TYR	L235	V236	
	D113	A175	LYS	V236	R237	
	L114	T176	TYR	R237	N238	
	Q115	G177	GLN	N238	K239	
	K116	I179		K239	N240	
	G117	N180		N240	K241	
	E118	M181				
	K119					

• Molecule 21: P19



TYR
ASP
TYR
LYS
PHE

● Molecule 21: P19

Chain cI:  74% 26%

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

T61 F62 S63 L64 M65 V66 P67 V68 N69 N70 S71 I72 A73 T74 I75 D76 F77 A78 E79 H80 N81 V82 G83 A84 V85 F86 K87 I88 E89 Y90 N91 R92 V93 N94 F95 I96 A97 P98 S99 L100 Y101 P102 I103 S104 G105 L106 G107 T108 V109 V111 F112 D113 Q115 K116 G117 E118 K119 A120

S121 Q122 R123 K124 I125 T126 E127 F128 G129 M130 K131 D132 I133 R134 I135 A136 D137 E138 I139 S140 D141 I142 A143 A144 D145 D146 H147 S148 V149 I150 I151 T152 T153 T154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 S165 R166 D167 V168 V169 N171 G172 E173 I174 A175 T176 G177 I178 I179 N180


M181 N182 T183 G184 F185 V186 S187 I188 D189 T189 I190 H191 T192 K193 K194 I195 S196 I197 T198 F198 V199 D200 G201 T202 V203 D204 Y205 Y206 V207 K208 I209 N210 V211 P212 T213 K214 Y215 S216 D217 G218 H218 I219 V220 E221 V222 V223 S224 G225 T226 F227 L228 N229 D230 I231 M232 T233 H234 L235 V236 K237 N238 K239 S300

K241 V242 A243 L244 M245 D246 S247 K248 Y249 T250 I251 V252 M253 N254 T255 N256 G257 F258 V259 T260 A261 K262 M263 P264 D265 D266 A267 M268 G269 V270 S271 L272 L273 K274 W275 W276 P277 R277 G278 A279 V280 V281 F282 P283 P284 Y285 V286 M287 T287 F288 K289 K290 F291 K292 N293 V294 N295 K296 W297 S298 I299 S300

Q301 Q302 I303 A304 S305 V307 N308 T309 S310 V311 K312 I313 P314 G315 G316 E317 Y318 S319 W320 K321 I322 R323 L324 F325 F326 G327 P328 I329 W330 Q331 V332 Q333 S334 S335 I336 N337 G338 V339 LYS THR VAL PRO HIS GLY ASN ASP THR MET TYR LEU TYR LYS GLU ILE VAL LYS TYR LYS

TYR
GLN
ASN
THR
LYS
ARG
ASN
PHE
GLU
HIS
TYR
ASP
TYR
ASP
LYS
PHE

● Molecule 21: P19

Chain cJ:  76% 23%

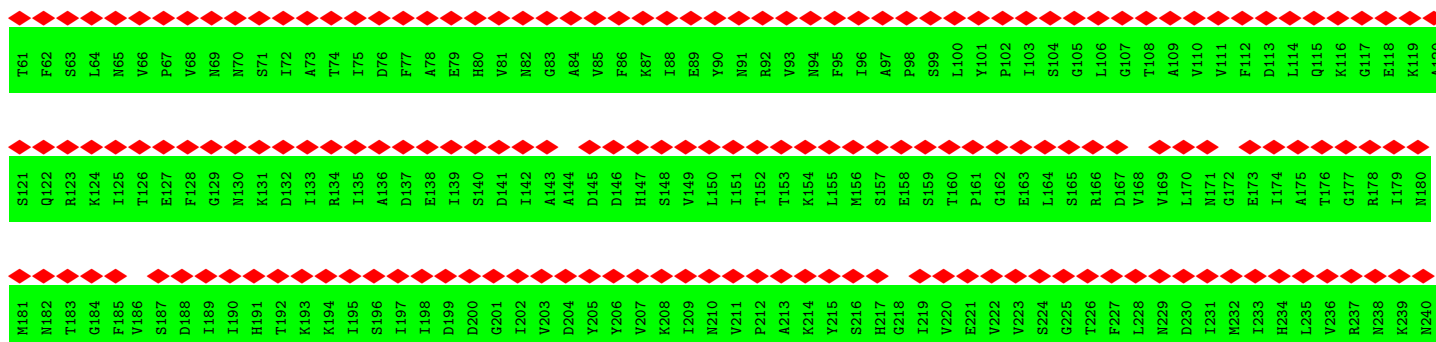
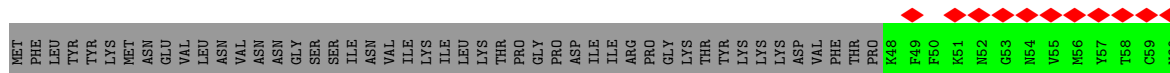
MET PHE LEU TYR TYR LYS MET ASN GLU VAL VAL ASN ASN GLY SER SER ILE ASN VAL ILE LYS LEU THR LYS THR PRO GLY PRO ASP ILE ILE ARG ARG GLY LYS THR TYR LYS LYS ASP VAL PHE THR PRO K48 F49 F50 K51 N52 Q53 N54 V55 M56 T58 C59 M60

T61 F62 S63 L64 M65 V66 P67 V68 N69 N70 S71 I72 A73 T74 I75 D76 F77 A78 E79 H80 N81 V82 G83 A84 V85 F86 K87 I88 E89 Y90 N91 R92 V93 N94 F95 I96 A97 P98 S99 L100 Y101 P102 I103 S104 G105 L106 G107 T108 V109 V111 F112 D113 Q115 K116 G117 E118 K119 A120

S121 Q122 R123 K124 I125 T126 E127 F128 G129 M130 K131 D132 I133 R134 I135 A136 D137 E138 I139 S140 D141 I142 D145 D146 H147 S148 V149 I150 I151 T152 T153 K154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 S165 R166 D167 V168 V169 N171 I174 A175 T176 G177 I178 I179 N180 M181 M182

T183 F185 V186 S187 D188 I189 T192 K193 K194 I195 S196 I197 T198 F198 V199 D200 G201 T202 V203 D204 Y205 Y206 V207 K208 I209 N210 V211 P212 A213 K214 Y215 S216 H217 L218 I219 V220 E221 V222 V223 S224 G225 T226 F227 L228 N229 D230 I231 M232 T233 H234 L235 V236 R237 N238 K239 N240 W241 W242 A243

L244 M245 D246 S247 K248 Y249 T250 I251 V252 M253 N254 T255 N256 G257 F258 V259 D260 A261 K262 M263 P264 D265 T266 A267 M268 G269 V270 S271 L272 L273 K274 W275 W276 P277 R277 G278 A279 V280 V281 F282 P283 P284 Y285 V286 M287 T287 F288 K289 K290 F291 K292 N293 V294 N295 K296 W297 S298 I299 S300 Q301 Q302 I303



K241	Q301	TYR
W242	Q302	GLN
A243	I303	PHE
L244	A304	LEU
M245	S305	THR
D246	C306	LYS
S247	V307	MET
K248	N308	ASN
M249	T309	VAL
Y250	S310	LEU
I251	V311	ASN
V252	K312	ASP
N253	A313	TYR
N254	S314	LYS
T255	I315	PHE
N256	G316	
G257	E317	
F258	Y318	
V259	S319	
I260	W320	
A261	K321	
K262	I322	
N263	R323	
P264	L324	
D265	F325	
T266	F326	
A267	G327	
M268	P328	
G269	I329	
V270	W330	
S271	Q331	
L272	V332	
L273	Q333	
E274	E334	
W275	S335	
P276	I336	
R277	N337	
G278	S338	
A279	V339	
V280	LYS	THR
V281	VAL	VAL
F282	ASN	PRO
P283	HIS	HIS
P284	GLY	VAL
Y285	ASN	GLY
Y286	ASP	ASP
N287	TYR	TYR
F288	MET	MET
K289	LEU	TYR
K290	LYS	LYS
F291	GLU	GLU
K292	ILE	ILE
N293	VAL	VAL
V294	LYS	LYS
N295	TYR	TYR
K296		
W297		
S298		
I299		
S300		

• Molecule 21: P19

Chain cM:



MET	THR	K241	Q301	TYR
PHE	PHE	W242	Q302	GLN
LEU	S63	A243	I303	ARG
THR	L64	L244	A304	ASN
LYS	N65	M245	S305	THR
MET	V66	D246	C306	LYS
ASN	P67	S247	V307	ARG
GLU	V68	K248	N308	ASN
VAL	N69	M249	T309	VAL
ASN	N70	Y250	S310	LEU
VAL	S71	I251	V311	ASN
ASN	I72	V252	K312	ASP
GLY	A73	N253	A313	TYR
SER	T74	N254	P314	LYS
ILE	I75	T255	G315	PHE
ASN	D76	N256	G316	
VAL	F77	G257	E317	
ILE	A78	F258	S319	
LYS	E79	V259	W320	
LEU	H80	I260	K321	
LYS	V81	A261	I322	
THR	N82	K262	R323	
PRO	G83	N263	L324	
GLY	A84	P264	D265	
PRO	V85	D266	T266	
ASP	F86	A267	G267	
ILE	K87	M268	P328	
ILE	I88	G269	I329	
ARG	E89	V270	W330	
ARG	Y90	S271	Q331	
GLY	N91	L272	V332	
LYS	R92	L273	Q333	
LYS	V93	E274	E334	
VAL	N94	W275	S335	
VAL	F95	P276	I336	
PHE	I96	R277	N337	
THR	A97	G278	S338	
LYS	P98	A279	V339	
PHE	S99	V280	LYS	THR
PHE	L100	V281	VAL	VAL
LYS	Y101	F282	ASN	PRO
ASN	P102	P283	HIS	HIS
ASN	I103	P284	GLY	VAL
VAL	S104	Y285	ASN	GLY
MET	G105	Y286	ASP	ASP
TYR	L106	N287	TYR	TYR
THR	G107	F288	MET	MET
CYS	T108	K289	LEU	TYR
ASN	A109	K290	LYS	LYS
	V110	F291	GLU	GLU
	V111	K292	ILE	ILE
	F112	N293	VAL	VAL
	D113	V294	LYS	LYS
	L114	N295	TYR	TYR
	Q115	K296		
	K116	W297		
	E118	S298		
	K119	I299		
	A120	S300		

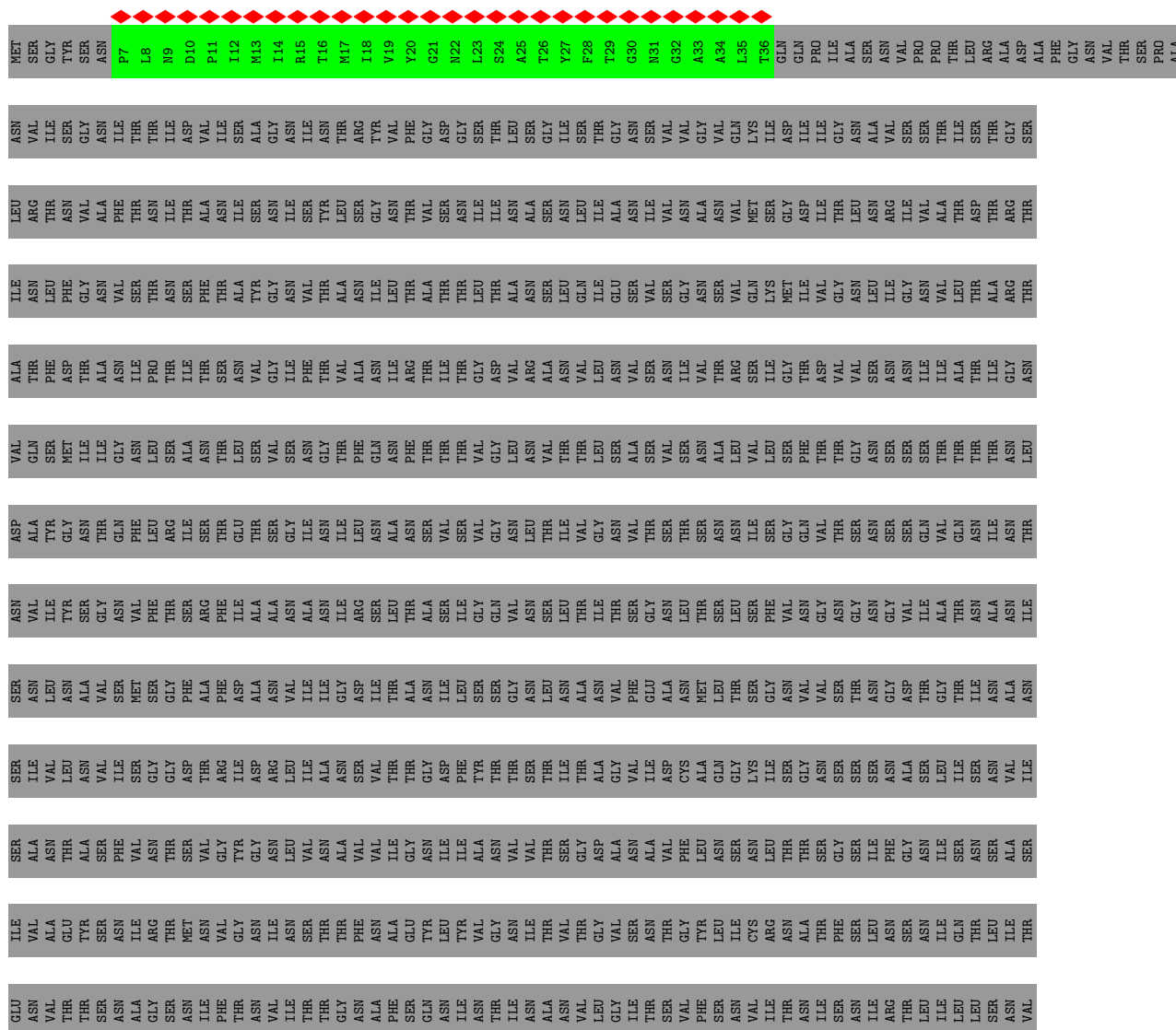
• Molecule 21: P19

Chain cN:



MET	T61	K48
PHE	F62	K51
LEU	S63	M52
TYR	L64	M53
LYS	N65	M54
MET	V66	M55
ASN	P67	M56
VAL	F68	Y57
GLU	N69	F58
LEU	N70	C59
ASN	S71	N60
VAL	I72	
ASN	A73	
GLY	T74	
SER	I75	
ILE	D76	
ASN	F77	
ASN	A78	
ILE	E79	
LEU	H80	
LYS	V81	
THR	N82	
PRO	G83	
GLY	A84	
PRO	D85	
ASP	F86	
ILE	K87	
ILE	I88	
ARG	E89	
ARG	Y90	
GLY	N91	
LYS	R92	
LYS	V93	
ASP	Q94	
VAL	N95	
PHE	I96	
THR	A97	
PRO	P98	
	F49	
	S99	
	L100	
	P101	
	G102	
	S103	
	I104	
	V105	
	G106	
	R107	
	T108	
	A109	
	V110	
	N111	
	F112	
	D113	
	I114	
	A115	
	T116	
	G117	
	E118	
	K119	
	I119	
	N180	

- Molecule 22: P20











- Molecule 23: P21

cP:  97%



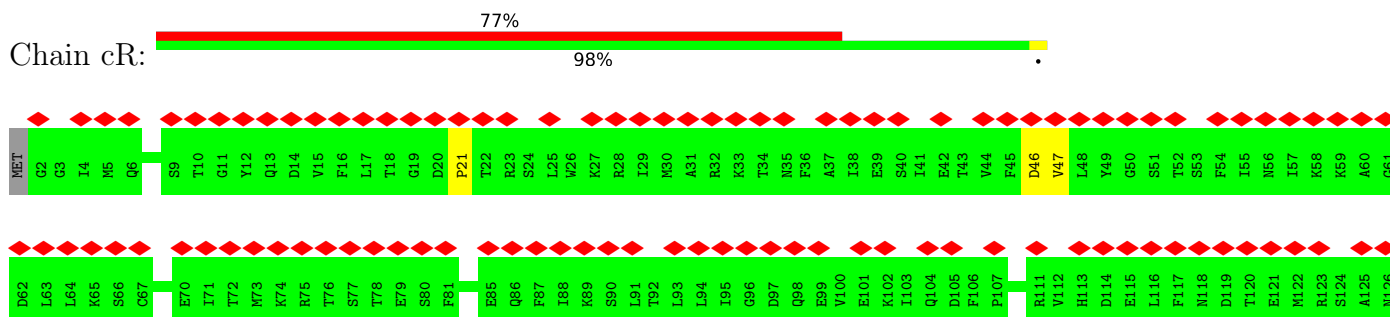
- Molecule 23: P21

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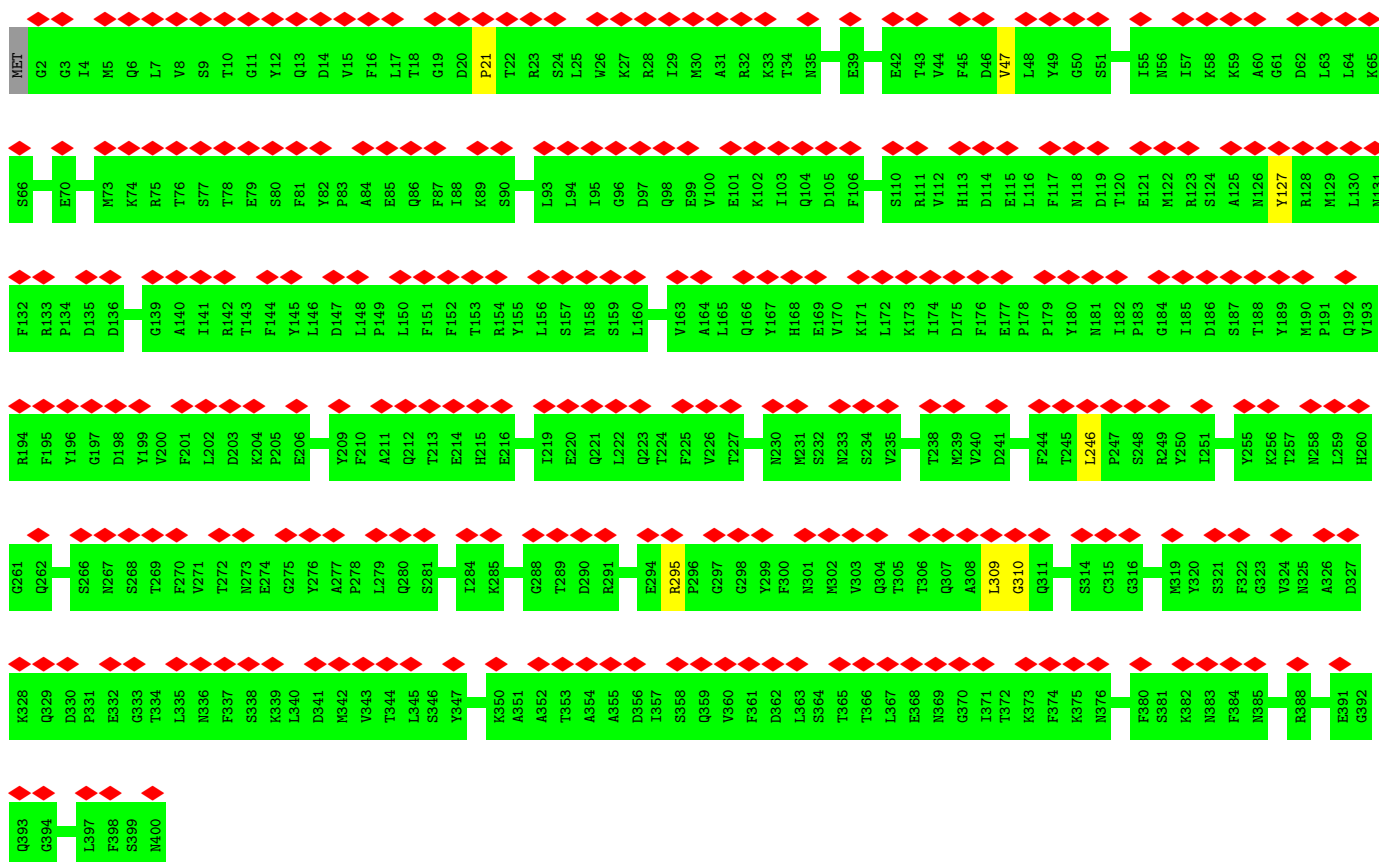
Chain dh:  97%

- Molecule 24: MCPv5

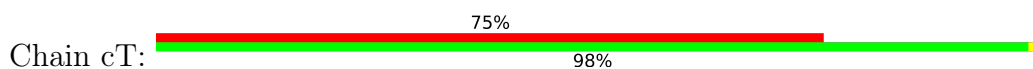




• Molecule 24: MCPv5



• Molecule 24: MCPv5



- Molecule 25: P22

[illegible]

- Molecule 25: P22

Chain cW:  97%

MET	GLY	SER	TYR	PHE	V6	A9	N10	Y11	F12	F13	K14	D15	I16	F17	A18	S19	N20	V21	G22	N23	I24	A25	N26	V27	I28	F29	D30	N31	G32	N33	V34	I35	A36	A37	G38	G39	L40	G41	Y42	L43	I44	G45	N46	G47	A48	PHE	ILE	THR	GLY	VAL	THR	SER	THR	ALA	ILE	ALA	ASN	ILE																																																																																																																																																																																																																																																																																																																																																																																																																				
PRO	ALA	VAL	THR	THR	ASP	ILE	ARG	GLY	LEU	ILE	GLY	TYR	ALA	ASN	VAL	ASN	ILE	ILE	ALA	SER	SER	GLY	ILE	SER	ASN	VAL	ARG	PHE	VAL	ASN	THR	ALA	SER	TYR	TYR	PHE	GLY	ASP	GLY	SER	GLN	LEU	THR	GLY	THR	ALA	THR	ALA	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																												
ILE	PRO	SER	ILE	VAL	THR	ASP	ILE	ARG	GLY	ILE	GLY	ASN	TYR	ALA	ASN	VAL	ASN	VAL	SER	SER	ALA	ASN	ILE	THR	PHE	ALA	ASN	PHE	ASN	ASN	THR	ALA	ALA	GLY	PHE	ASN	PHE	ILE	GLY	ASN	LEU	LEU	THR	THR	ALA	THR	GLY	ILE	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																												
ALA	THR	ALA	ASN	ILE	PRO	ILE	VAL	THR	ALA	ASP	ILE	ILE	ILE	GLY	GLY	TYR	ASN	ASN	VAL	SER	THR	ALA	ASN	THR	PHE	ILE	ALA	ASN	ASN	VAL	ASN	GLY	PHE	ASN	ASN	GLY	THR	ASN	GLY	ASN	THR	THR	GLY	THR	ASN	GLY	THR	ALA	LEU	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																											
THR	GLY	ILE	THR	THR	ALA	THR	ALA	GLN	THR	PRO	VAL	ILE	THR	THR	ALA	ASP	ILE	ASN	THR	ASP	ILE	ILE	ILE	ALA	GLY	VAL	THR	THR	VAL	ASN	ALA	THR	PHE	ASN	ASN	GLY	THR	ASN	GLY	THR	ASN	VAL	THR	THR	ALA	THR	GLY	THR	ALA	LEU	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																										
GLY	ASN	GLY	THR	PHE	GLY	ASN	GLY	GLN	LEU	GLY	VAL	THR	ALA	THR	LEU	PRO	SER	ILE	THR	ASP	ILE	ILE	ILE	GLY	ASN	VAL	THR	ALA	TYR	ASN	VAL	ALA	PHE	GLY	ASN	ILE	ASN	ASN	VAL	LEU	PHE	ASN	GLY	THR	ALA	THR	VAL	THR	ASN	GLY	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																										
PHE	ILE	GLY	ASN	GLY	ASN	THR	PHE	GLY	GLN	THR	VAL	THR	ILE	PRO	LEU	THR	ALA	VAL	THR	ALA	ILE	ARG	ILE	GLY	ASN	VAL	THR	GLY	ASN	VAL	ASN	THR	ALA	ASN	THR	ILE	ASN	ASN	VAL	LEU	PHE	ASN	GLY	THR	ALA	THR	VAL	THR	ASN	GLY	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																										
ALA	ASP	GLY	ASN	GLY	THR	PHE	ASN	GLY	GLY	LEU	THR	VAL	VAL	THR	ALA	THR	PRO	VAL	THR	ALA	ILE	THR	ASN	THR	ALA	THR	ASP	GLY	ASN	VAL	ASN	ALA	THR	PHE	GLY	ASN	ASN	VAL	LEU	THR	ASN	VAL	THR	THR	ALA	THR	VAL	THR	ASN	GLY	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																										
THR	ALA	ALA	GLY	GLY	ASN	GLY	PHE	GLY	ASN	GLY	LEU	THR	THR	GLY	ILE	THR	ALA	ALA	ASN	THR	ALA	VAL	THR	ALA	ALA	ASP	GLY	ASN	ILE	THR	ASN	VAL	ASN	THR	ALA	THR	ILE	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																								
ASN	GLY	ASN	VAL	THR	ALA	ASP	GLY	TYR	PHE	GLY	GLY	GLY	GLY	THR	ASN	GLN	GLY	THR	THR	ALA	THR	THR	ILE	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																						
PHE	ASN	ASN	GLY	ASN	VAL	THR	ALA	GLY	THR	PHE	GLY	GLY	GLY	ALA	GLY	ALA	THR	THR	GLY	THR	ALA	THR	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																			
ALA	ASN	VAL	PHE	ASN	ASN	GLY	ASN	VAL	ALA	GLY	THR	GLY	GLY	THR	ALA	THR	ASN	GLY	THR	ILE	THR	ASN	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																		
ASN	ILE	ALA	ASN	VAL	LEU	PHE	ASN	GLY	THR	ALA	GLY	GLY	GLY	ALA	THR	ALA	THR	TYR	PHE	GLY	THR	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																															
THR	TYR	SER	THR	GLY	ASN	ILE	ASN	VAL	PHE	ASN	ASN	VAL	THR	ALA	ALA	GLY	ASN	GLY	TYR	PHE	THR	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56500	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 ($e^-/\text{\AA}^2$)	24.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.269	Depositor
Minimum map value	-1.541	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	1944.0, 1944.0, 1944.0	wwPDB
Map dimensions	1200, 1200, 1200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.62, 1.62, 1.62	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	aA	0.55	0/3468	0.69	0/4728
1	aB	0.58	0/3468	0.71	0/4728
1	aC	0.58	0/3473	0.71	0/4735
1	aD	0.60	0/3460	0.76	0/4717
1	aE	0.57	0/3473	0.72	0/4735
1	aF	0.58	0/3460	0.70	0/4717
1	aG	0.56	0/3468	0.70	0/4728
1	aH	0.55	0/3460	0.72	0/4717
1	aI	0.57	0/3468	0.71	0/4728
1	aJ	0.58	0/3473	0.70	0/4735
1	aK	0.55	0/3473	0.74	1/4735 (0.0%)
1	aL	0.58	0/3465	0.73	0/4724
1	aM	0.57	0/3473	0.71	0/4735
1	aN	0.58	0/3468	0.71	0/4728
1	aO	0.57	0/3473	0.72	0/4735
1	aP	0.57	0/3473	0.71	0/4735
1	aQ	0.58	0/3460	0.72	0/4717
1	aR	0.58	0/3473	0.73	0/4735
1	aS	0.57	0/3473	0.71	0/4735
1	aT	0.58	0/3473	0.70	0/4735
1	aU	0.58	0/3473	0.70	0/4735
1	aV	0.56	0/3473	0.69	0/4735
1	aW	0.56	0/3473	0.71	0/4735
1	aX	0.58	0/3468	0.72	0/4728
1	aY	0.57	0/3473	0.71	0/4735
1	aZ	0.57	0/3473	0.71	0/4735
1	aa	0.84	0/3452	0.83	0/4707
1	ab	0.88	0/3473	0.88	0/4735
1	ac	0.83	0/3473	0.82	1/4735 (0.0%)
1	ad	0.57	0/3473	0.71	1/4735 (0.0%)
1	ae	0.56	0/3473	0.69	0/4735
1	af	0.57	0/3473	0.71	0/4735
1	ag	0.57	0/3473	0.70	0/4735
1	ah	0.56	0/3473	0.70	0/4735

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ai	0.56	0/3473	0.71	0/4735
1	aj	0.57	0/3473	0.70	0/4735
1	ak	0.56	0/3473	0.69	0/4735
1	al	0.55	0/3465	0.72	0/4724
1	am	0.57	0/3473	0.73	0/4735
1	an	0.57	0/3465	0.69	0/4724
1	ao	0.57	0/3468	0.71	0/4728
1	ap	0.57	0/3473	0.72	0/4735
1	aq	0.56	0/3473	0.72	0/4735
1	ar	0.57	0/3460	0.72	0/4717
1	as	0.56	0/3473	0.69	0/4735
1	at	0.56	0/3473	0.69	0/4735
1	au	0.56	0/3460	0.70	0/4717
1	av	0.54	0/3473	0.70	0/4735
1	aw	0.56	0/3473	0.72	0/4735
1	ax	0.56	0/3460	0.69	0/4717
1	ay	0.57	0/3468	0.69	0/4728
1	az	0.57	0/3460	0.69	0/4717
1	ba	0.58	0/3473	0.73	0/4735
1	bb	0.56	0/3473	0.69	0/4735
1	bc	0.58	0/3473	0.72	0/4735
1	bd	0.57	0/3473	0.71	0/4735
1	be	0.57	0/3473	0.71	0/4735
1	bf	0.56	0/3473	0.73	0/4735
1	bg	0.57	0/3473	0.70	0/4735
1	bh	0.57	0/3473	0.69	0/4735
1	bi	0.57	0/3473	0.71	0/4735
1	bj	0.56	0/3473	0.69	0/4735
1	bk	0.56	0/3473	0.69	0/4735
1	bl	0.57	0/3473	0.69	0/4735
1	bm	0.57	0/3473	0.73	0/4735
1	bn	0.56	0/3460	0.70	0/4717
1	bo	0.58	0/3473	0.70	0/4735
1	bp	0.58	0/3473	0.74	0/4735
1	bq	0.58	0/3473	0.71	0/4735
1	br	0.58	0/3473	0.71	0/4735
1	bs	0.58	0/3473	0.70	0/4735
1	bt	0.57	0/3468	0.71	0/4728
2	bA	0.59	0/4196	0.71	0/5743
2	bB	0.60	0/4208	0.60	0/5759
2	bu	0.81	0/4208	0.80	0/5759
2	bv	0.79	0/4208	0.79	0/5759
2	bw	0.80	0/4208	0.81	0/5759

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	bx	0.80	0/4191	0.82	0/5736
2	by	0.78	0/4208	0.79	0/5759
2	bz	0.79	0/4147	0.81	0/5676
3	bC	0.59	0/4020	0.55	0/5461
4	bD	0.61	0/3248	0.69	0/4423
4	bF	0.61	0/3248	0.68	0/4423
4	cX	0.60	0/3244	0.71	0/4418
4	cZ	0.61	0/3244	0.71	0/4418
4	dd	0.61	0/3248	0.70	0/4423
4	df	0.61	0/3244	0.71	0/4418
4	dj	0.62	0/3248	0.71	0/4423
4	dk	0.60	0/3248	0.70	0/4423
4	dl	0.61	0/3248	0.71	0/4423
4	dp	0.60	0/3248	0.70	0/4423
4	dr	0.62	0/3248	0.71	0/4423
5	bE	0.61	0/3218	0.69	0/4365
5	cY	0.61	0/3218	0.69	1/4365 (0.0%)
5	de	0.61	0/3218	0.69	1/4365 (0.0%)
5	dq	0.61	0/3218	0.69	1/4365 (0.0%)
6	bG	0.62	0/3957	0.56	0/5413
7	bH	0.62	0/3333	0.72	0/4542
8	bI	0.67	0/1120	0.77	0/1517
8	bJ	0.67	0/1172	0.80	0/1590
8	bK	0.66	0/909	0.78	0/1228
9	bL	0.65	0/537	0.79	0/720
9	bM	0.64	0/537	0.78	0/720
9	bN	0.63	0/530	0.84	0/710
9	bO	0.62	0/530	0.76	0/710
10	bP	0.77	0/1155	0.76	0/1573
11	bQ	0.70	0/1307	0.81	0/1775
12	bR	0.72	0/1270	0.67	0/1716
13	bS	0.26	0/1534	0.61	1/2075 (0.0%)
14	bT	0.52	0/382	0.94	0/520
14	bU	0.58	0/436	0.80	0/596
14	bV	0.51	0/428	0.75	0/585
14	bW	0.51	0/416	0.73	0/569
14	bX	0.53	0/319	0.84	0/435
14	bY	0.63	0/593	0.87	0/810
14	bZ	0.54	0/416	0.74	0/569
14	ca	0.51	0/416	0.78	0/569
14	cb	0.61	0/416	0.89	0/569
14	cc	0.56	0/665	0.77	1/911 (0.1%)
14	cd	0.60	0/601	0.83	1/821 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
14	ce	0.61	0/576	0.73	0/787
15	cf	0.70	0/647	0.72	0/873
16	cg	0.68	0/535	0.79	0/723
17	ch	0.77	0/1319	0.79	0/1781
18	ci	0.42	0/565	0.66	1/760 (0.1%)
19	cj	0.27	0/471	0.54	0/643
19	ck	0.25	0/464	0.50	0/629
19	cl	0.27	0/438	0.51	0/595
19	cm	0.25	0/513	0.55	0/697
20	cn	0.26	0/778	0.53	0/1051
20	co	0.26	0/744	0.53	0/1010
21	cA	0.59	0/2239	0.53	0/3040
21	cB	0.61	0/2350	0.59	0/3188
21	cC	0.60	0/2239	0.54	0/3040
21	cD	0.59	0/2350	0.56	0/3188
21	cE	0.60	0/2247	0.57	0/3051
21	cF	0.61	0/2350	0.58	0/3188
21	cG	0.60	0/2260	0.56	0/3069
21	cH	0.63	0/2350	0.60	0/3188
21	cI	0.59	0/2239	0.56	0/3040
21	cJ	0.61	0/2350	0.58	0/3188
21	cK	0.60	0/2239	0.54	0/3040
21	cL	0.60	0/2350	0.59	0/3188
21	cM	0.59	0/2220	0.54	0/3014
21	cN	0.58	0/2350	0.56	0/3188
21	cp	0.60	0/2350	0.57	0/3188
21	cq	0.59	0/2260	0.55	0/3069
21	cr	0.60	0/2350	0.56	0/3188
21	cs	0.60	0/2206	0.55	0/2995
21	ct	0.60	0/2350	0.56	0/3188
21	cu	0.59	0/2247	0.52	0/3051
21	cv	0.61	0/2350	0.60	0/3188
21	cw	0.63	0/2247	0.57	0/3051
21	cx	0.63	0/2350	0.59	0/3188
21	cy	0.61	0/2247	0.56	0/3051
21	cz	0.59	0/2350	0.56	0/3188
22	cO	0.48	0/222	0.70	0/302
22	cQ	0.44	0/237	0.57	0/322
22	da	0.38	0/231	0.59	0/316
22	dc	0.43	0/213	0.57	0/289
22	dg	0.38	0/245	0.52	0/334
22	di	0.37	0/215	0.58	0/293
22	ds	0.35	0/242	0.53	0/330

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	du	0.34	0/228	0.55	0/310
23	cP	0.41	0/244	0.55	0/333
23	db	0.42	0/203	0.57	0/277
23	dh	0.36	0/254	0.59	0/345
23	dt	0.29	0/239	0.54	0/324
24	cR	0.65	0/3281	0.72	2/4457 (0.0%)
24	cS	0.65	0/3281	0.72	2/4457 (0.0%)
24	cT	0.64	0/3281	0.72	2/4457 (0.0%)
25	cU	0.35	0/318	0.57	0/433
25	cV	0.34	0/312	0.56	0/425
25	cW	0.37	0/315	0.54	0/429
26	dm	0.41	0/176	0.63	0/243
26	dn	0.40	0/183	0.57	0/252
26	do	0.39	0/185	0.69	1/255 (0.4%)
All	All	0.60	0/437605	0.70	17/596073 (0.0%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	bS	27	ILE	C-N-CD	-13.89	90.05	120.60
18	ci	35	TRP	C-N-CD	-6.33	106.67	120.60
24	cT	127	TYR	CA-CB-CG	5.85	124.52	113.40
24	cS	127	TYR	CA-CB-CG	5.84	124.50	113.40
24	cR	127	TYR	CA-CB-CG	5.83	124.48	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	3390	0	3284	0	0
1	aB	3390	0	3284	0	0
1	aC	3395	0	3289	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aD	3382	0	3278	0	0
1	aE	3395	0	3289	0	0
1	aF	3382	0	3278	0	0
1	aG	3390	0	3284	0	0
1	aH	3382	0	3278	0	0
1	aI	3390	0	3284	0	0
1	aJ	3395	0	3289	0	0
1	aK	3395	0	3289	0	0
1	aL	3387	0	3283	0	0
1	aM	3395	0	3289	0	0
1	aN	3390	0	3284	0	0
1	aO	3395	0	3289	0	0
1	aP	3395	0	3289	0	0
1	aQ	3382	0	3278	0	0
1	aR	3395	0	3289	0	0
1	aS	3395	0	3289	0	0
1	aT	3395	0	3289	0	0
1	aU	3395	0	3289	0	0
1	aV	3395	0	3289	0	0
1	aW	3395	0	3289	0	0
1	aX	3390	0	3284	0	0
1	aY	3395	0	3289	0	0
1	aZ	3395	0	3289	0	0
1	aa	3374	0	3272	0	0
1	ab	3395	0	3289	0	0
1	ac	3395	0	3289	0	0
1	ad	3395	0	3289	0	0
1	ae	3395	0	3289	0	0
1	af	3395	0	3289	0	0
1	ag	3395	0	3289	0	0
1	ah	3395	0	3289	0	0
1	ai	3395	0	3289	0	0
1	aj	3395	0	3289	0	0
1	ak	3395	0	3289	0	0
1	al	3387	0	3283	0	0
1	am	3395	0	3289	0	0
1	an	3387	0	3283	0	0
1	ao	3390	0	3284	0	0
1	ap	3395	0	3289	0	0
1	aq	3395	0	3289	0	0
1	ar	3382	0	3278	0	0
1	as	3395	0	3289	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	at	3395	0	3289	0	0
1	au	3382	0	3278	0	0
1	av	3395	0	3289	0	0
1	aw	3395	0	3289	0	0
1	ax	3382	0	3278	0	0
1	ay	3390	0	3284	0	0
1	az	3382	0	3278	0	0
1	ba	3395	0	3289	0	0
1	bb	3395	0	3289	0	0
1	bc	3395	0	3289	0	0
1	bd	3395	0	3289	0	0
1	be	3395	0	3289	0	0
1	bf	3395	0	3289	0	0
1	bg	3395	0	3289	0	0
1	bh	3395	0	3289	0	0
1	bi	3395	0	3289	0	0
1	bj	3395	0	3289	0	0
1	bk	3395	0	3289	0	0
1	bl	3395	0	3289	0	0
1	bm	3395	0	3289	0	0
1	bn	3382	0	3278	0	0
1	bo	3395	0	3289	0	0
1	bp	3395	0	3289	0	0
1	bq	3395	0	3289	0	0
1	br	3395	0	3289	0	0
1	bs	3395	0	3289	0	0
1	bt	3390	0	3284	0	0
2	bA	4079	0	3911	0	0
2	bB	4090	0	3920	0	0
2	bu	4090	0	3920	0	0
2	bv	4090	0	3920	0	0
2	bw	4090	0	3920	0	0
2	bx	4074	0	3904	0	0
2	by	4090	0	3920	0	0
2	bz	4030	0	3855	0	0
3	bC	3921	0	3830	0	0
4	bD	3169	0	3084	0	0
4	bF	3169	0	3084	0	0
4	cX	3165	0	3080	0	0
4	cZ	3165	0	3080	0	0
4	dd	3169	0	3084	0	0
4	df	3165	0	3080	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	dj	3169	0	3084	0	0
4	dk	3169	0	3084	0	0
4	dl	3169	0	3084	0	0
4	dp	3169	0	3084	0	0
4	dr	3169	0	3084	0	0
5	bE	3146	0	3091	0	0
5	cY	3146	0	3091	0	0
5	de	3146	0	3091	0	0
5	dq	3146	0	3091	0	0
6	bG	3864	0	3724	0	0
7	bH	3258	0	3136	0	0
8	bI	1096	0	1079	0	0
8	bJ	1146	0	1125	0	0
8	bK	892	0	879	0	0
9	bL	526	0	535	0	0
9	bM	526	0	535	0	0
9	bN	519	0	528	0	0
9	bO	519	0	528	0	0
10	bP	1126	0	1142	0	0
11	bQ	1275	0	1274	0	0
12	bR	1244	0	1254	0	0
13	bS	1504	0	1497	0	0
14	bT	373	0	370	0	0
14	bU	424	0	415	0	0
14	bV	416	0	409	0	0
14	bW	405	0	400	0	0
14	bX	312	0	301	0	0
14	bY	576	0	561	0	0
14	bZ	405	0	400	0	0
14	ca	405	0	400	0	0
14	cb	405	0	400	0	0
14	cc	646	0	643	0	0
14	cd	583	0	569	0	0
14	ce	560	0	541	0	0
15	cf	631	0	625	0	0
16	cg	521	0	494	0	0
17	ch	1288	0	1280	0	0
18	ci	553	0	539	0	0
19	cj	463	0	449	0	0
19	ck	455	0	448	0	0
19	cl	431	0	422	0	0
19	cm	503	0	486	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	cn	769	0	785	0	0
20	co	733	0	728	0	0
21	cA	2191	0	2203	0	0
21	cB	2299	0	2307	0	0
21	cC	2191	0	2203	0	0
21	cD	2299	0	2307	0	0
21	cE	2199	0	2209	0	0
21	cF	2299	0	2307	0	0
21	cG	2212	0	2221	0	0
21	cH	2299	0	2307	0	0
21	cI	2191	0	2203	0	0
21	cJ	2299	0	2307	0	0
21	cK	2191	0	2203	0	0
21	cL	2299	0	2307	0	0
21	cM	2173	0	2187	0	0
21	cN	2299	0	2307	0	0
21	cp	2299	0	2307	0	0
21	cq	2212	0	2221	0	0
21	cr	2299	0	2307	0	0
21	cs	2159	0	2171	0	0
21	ct	2299	0	2307	0	0
21	cu	2199	0	2209	0	0
21	cv	2299	0	2307	0	0
21	cw	2199	0	2209	0	0
21	cx	2299	0	2307	0	0
21	cy	2199	0	2209	0	0
21	cz	2299	0	2307	0	0
22	cO	218	0	220	0	0
22	cQ	233	0	234	0	0
22	da	228	0	221	0	0
22	dc	209	0	208	0	0
22	dg	241	0	239	0	0
22	di	211	0	208	0	0
22	ds	238	0	237	0	0
22	du	224	0	226	0	0
23	cP	239	0	226	0	0
23	db	200	0	188	0	0
23	dh	249	0	241	0	0
23	dt	236	0	229	0	0
24	cR	3203	0	3142	0	0
24	cS	3203	0	3142	0	0
24	cT	3203	0	3142	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	cU	311	0	299	0	0
25	cV	305	0	293	0	0
25	cW	308	0	297	0	0
26	dm	174	0	154	0	0
26	dn	181	0	169	0	0
26	do	182	0	175	0	0
All	All	427569	0	416835	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

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	aA	433/437 (99%)	421 (97%)	12 (3%)	0	100	100
1	aB	433/437 (99%)	424 (98%)	9 (2%)	0	100	100
1	aC	434/437 (99%)	423 (98%)	11 (2%)	0	100	100
1	aD	432/437 (99%)	421 (98%)	11 (2%)	0	100	100
1	aE	434/437 (99%)	419 (96%)	15 (4%)	0	100	100
1	aF	432/437 (99%)	421 (98%)	11 (2%)	0	100	100
1	aG	433/437 (99%)	420 (97%)	13 (3%)	0	100	100
1	aH	432/437 (99%)	422 (98%)	9 (2%)	1 (0%)	47	79
1	aI	433/437 (99%)	422 (98%)	10 (2%)	1 (0%)	47	79
1	aJ	434/437 (99%)	421 (97%)	13 (3%)	0	100	100
1	aK	434/437 (99%)	420 (97%)	12 (3%)	2 (0%)	29	66
1	aL	433/437 (99%)	419 (97%)	13 (3%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aM	434/437 (99%)	418 (96%)	16 (4%)	0	100	100
1	aN	433/437 (99%)	419 (97%)	13 (3%)	1 (0%)	47	79
1	aO	434/437 (99%)	419 (96%)	14 (3%)	1 (0%)	47	79
1	aP	434/437 (99%)	422 (97%)	11 (2%)	1 (0%)	47	79
1	aQ	432/437 (99%)	420 (97%)	11 (2%)	1 (0%)	47	79
1	aR	434/437 (99%)	416 (96%)	14 (3%)	4 (1%)	17	54
1	aS	434/437 (99%)	418 (96%)	15 (4%)	1 (0%)	47	79
1	aT	434/437 (99%)	417 (96%)	15 (4%)	2 (0%)	29	66
1	aU	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	47	79
1	aV	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	47	79
1	aW	434/437 (99%)	420 (97%)	14 (3%)	0	100	100
1	aX	433/437 (99%)	420 (97%)	13 (3%)	0	100	100
1	aY	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	47	79
1	aZ	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	47	79
1	aa	430/437 (98%)	420 (98%)	10 (2%)	0	100	100
1	ab	434/437 (99%)	430 (99%)	4 (1%)	0	100	100
1	ac	434/437 (99%)	425 (98%)	9 (2%)	0	100	100
1	ad	434/437 (99%)	419 (96%)	13 (3%)	2 (0%)	29	66
1	ae	434/437 (99%)	419 (96%)	15 (4%)	0	100	100
1	af	434/437 (99%)	422 (97%)	12 (3%)	0	100	100
1	ag	434/437 (99%)	415 (96%)	19 (4%)	0	100	100
1	ah	434/437 (99%)	417 (96%)	16 (4%)	1 (0%)	47	79
1	ai	434/437 (99%)	418 (96%)	16 (4%)	0	100	100
1	aj	434/437 (99%)	423 (98%)	11 (2%)	0	100	100
1	ak	434/437 (99%)	422 (97%)	10 (2%)	2 (0%)	29	66
1	al	433/437 (99%)	425 (98%)	7 (2%)	1 (0%)	47	79
1	am	434/437 (99%)	423 (98%)	11 (2%)	0	100	100
1	an	433/437 (99%)	423 (98%)	10 (2%)	0	100	100
1	ao	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	ap	434/437 (99%)	417 (96%)	17 (4%)	0	100	100
1	aq	434/437 (99%)	425 (98%)	8 (2%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ar	432/437 (99%)	420 (97%)	12 (3%)	0	100	100
1	as	434/437 (99%)	418 (96%)	14 (3%)	2 (0%)	29	66
1	at	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	47	79
1	au	432/437 (99%)	421 (98%)	11 (2%)	0	100	100
1	av	434/437 (99%)	425 (98%)	9 (2%)	0	100	100
1	aw	434/437 (99%)	418 (96%)	15 (4%)	1 (0%)	47	79
1	ax	432/437 (99%)	417 (96%)	14 (3%)	1 (0%)	47	79
1	ay	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	az	432/437 (99%)	420 (97%)	12 (3%)	0	100	100
1	ba	434/437 (99%)	416 (96%)	17 (4%)	1 (0%)	47	79
1	bb	434/437 (99%)	420 (97%)	12 (3%)	2 (0%)	29	66
1	bc	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	47	79
1	bd	434/437 (99%)	423 (98%)	9 (2%)	2 (0%)	29	66
1	be	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	47	79
1	bf	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	47	79
1	bg	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	47	79
1	bh	434/437 (99%)	422 (97%)	11 (2%)	1 (0%)	47	79
1	bi	434/437 (99%)	419 (96%)	14 (3%)	1 (0%)	47	79
1	bj	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	47	79
1	bk	434/437 (99%)	419 (96%)	14 (3%)	1 (0%)	47	79
1	bl	434/437 (99%)	418 (96%)	15 (4%)	1 (0%)	47	79
1	bm	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	47	79
1	bn	432/437 (99%)	416 (96%)	15 (4%)	1 (0%)	47	79
1	bo	434/437 (99%)	419 (96%)	13 (3%)	2 (0%)	29	66
1	bp	434/437 (99%)	422 (97%)	11 (2%)	1 (0%)	47	79
1	bq	434/437 (99%)	420 (97%)	14 (3%)	0	100	100
1	br	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	47	79
1	bs	434/437 (99%)	421 (97%)	13 (3%)	0	100	100
1	bt	433/437 (99%)	423 (98%)	9 (2%)	1 (0%)	47	79
2	bA	514/520 (99%)	486 (95%)	26 (5%)	2 (0%)	34	70
2	bB	515/520 (99%)	480 (93%)	34 (7%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	bu	515/520 (99%)	489 (95%)	25 (5%)	1 (0%)	47	79
2	bv	515/520 (99%)	485 (94%)	29 (6%)	1 (0%)	47	79
2	bw	515/520 (99%)	490 (95%)	25 (5%)	0	100	100
2	bx	512/520 (98%)	483 (94%)	27 (5%)	2 (0%)	34	70
2	by	515/520 (99%)	482 (94%)	32 (6%)	1 (0%)	47	79
2	bz	506/520 (97%)	473 (94%)	32 (6%)	1 (0%)	47	79
3	bC	483/486 (99%)	459 (95%)	22 (5%)	2 (0%)	34	70
4	bD	399/403 (99%)	383 (96%)	14 (4%)	2 (0%)	29	66
4	bF	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
4	cX	399/403 (99%)	380 (95%)	14 (4%)	5 (1%)	12	48
4	cZ	399/403 (99%)	380 (95%)	14 (4%)	5 (1%)	12	48
4	dd	399/403 (99%)	379 (95%)	15 (4%)	5 (1%)	12	48
4	df	399/403 (99%)	377 (94%)	14 (4%)	8 (2%)	7	41
4	dj	399/403 (99%)	376 (94%)	20 (5%)	3 (1%)	19	57
4	dk	399/403 (99%)	374 (94%)	22 (6%)	3 (1%)	19	57
4	dl	399/403 (99%)	374 (94%)	20 (5%)	5 (1%)	12	48
4	dp	399/403 (99%)	381 (96%)	14 (4%)	4 (1%)	15	52
4	dr	399/403 (99%)	378 (95%)	14 (4%)	7 (2%)	8	42
5	bE	395/401 (98%)	382 (97%)	12 (3%)	1 (0%)	41	74
5	cY	395/401 (98%)	382 (97%)	12 (3%)	1 (0%)	41	74
5	de	395/401 (98%)	385 (98%)	10 (2%)	0	100	100
5	dq	395/401 (98%)	384 (97%)	10 (2%)	1 (0%)	41	74
6	bG	496/530 (94%)	478 (96%)	17 (3%)	1 (0%)	47	79
7	bH	422/576 (73%)	388 (92%)	32 (8%)	2 (0%)	29	66
8	bI	139/171 (81%)	131 (94%)	7 (5%)	1 (1%)	22	60
8	bJ	145/171 (85%)	135 (93%)	9 (6%)	1 (1%)	22	60
8	bK	114/171 (67%)	111 (97%)	3 (3%)	0	100	100
9	bL	61/181 (34%)	59 (97%)	1 (2%)	1 (2%)	9	44
9	bM	61/181 (34%)	55 (90%)	5 (8%)	1 (2%)	9	44
9	bN	60/181 (33%)	56 (93%)	3 (5%)	1 (2%)	9	43
9	bO	60/181 (33%)	54 (90%)	5 (8%)	1 (2%)	9	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	bP	140/146 (96%)	133 (95%)	7 (5%)	0	100	100
11	bQ	160/216 (74%)	149 (93%)	8 (5%)	3 (2%)	8	42
12	bR	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
13	bS	189/210 (90%)	172 (91%)	15 (8%)	2 (1%)	14	51
14	bT	46/207 (22%)	40 (87%)	3 (6%)	3 (6%)	1	19
14	bU	52/207 (25%)	48 (92%)	3 (6%)	1 (2%)	8	42
14	bV	51/207 (25%)	42 (82%)	8 (16%)	1 (2%)	7	41
14	bW	50/207 (24%)	45 (90%)	4 (8%)	1 (2%)	7	41
14	bX	39/207 (19%)	34 (87%)	4 (10%)	1 (3%)	5	36
14	bY	72/207 (35%)	58 (81%)	10 (14%)	4 (6%)	2	21
14	bZ	50/207 (24%)	46 (92%)	4 (8%)	0	100	100
14	ca	50/207 (24%)	47 (94%)	2 (4%)	1 (2%)	7	41
14	cb	50/207 (24%)	45 (90%)	4 (8%)	1 (2%)	7	41
14	cc	82/207 (40%)	73 (89%)	8 (10%)	1 (1%)	13	50
14	cd	73/207 (35%)	66 (90%)	7 (10%)	0	100	100
14	ce	70/207 (34%)	63 (90%)	6 (9%)	1 (1%)	11	46
15	cf	76/151 (50%)	67 (88%)	7 (9%)	2 (3%)	5	36
16	cg	64/98 (65%)	58 (91%)	3 (5%)	3 (5%)	2	24
17	ch	150/155 (97%)	143 (95%)	5 (3%)	2 (1%)	12	48
18	ci	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	12	48
19	cj	57/80 (71%)	51 (90%)	6 (10%)	0	100	100
19	ck	55/80 (69%)	52 (94%)	3 (6%)	0	100	100
19	cl	53/80 (66%)	51 (96%)	2 (4%)	0	100	100
19	cm	61/80 (76%)	58 (95%)	3 (5%)	0	100	100
20	cn	96/148 (65%)	93 (97%)	3 (3%)	0	100	100
20	co	93/148 (63%)	87 (94%)	6 (6%)	0	100	100
21	cA	277/378 (73%)	254 (92%)	23 (8%)	0	100	100
21	cB	290/378 (77%)	267 (92%)	23 (8%)	0	100	100
21	cC	277/378 (73%)	250 (90%)	26 (9%)	1 (0%)	34	70
21	cD	290/378 (77%)	267 (92%)	20 (7%)	3 (1%)	15	52
21	cE	278/378 (74%)	255 (92%)	21 (8%)	2 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	cF	290/378 (77%)	257 (89%)	30 (10%)	3 (1%)	15	52
21	cG	280/378 (74%)	253 (90%)	26 (9%)	1 (0%)	34	70
21	cH	290/378 (77%)	261 (90%)	28 (10%)	1 (0%)	41	74
21	cI	277/378 (73%)	256 (92%)	21 (8%)	0	100	100
21	cJ	290/378 (77%)	263 (91%)	24 (8%)	3 (1%)	15	52
21	cK	277/378 (73%)	258 (93%)	18 (6%)	1 (0%)	34	70
21	cL	290/378 (77%)	265 (91%)	24 (8%)	1 (0%)	41	74
21	cM	275/378 (73%)	252 (92%)	22 (8%)	1 (0%)	34	70
21	cN	290/378 (77%)	267 (92%)	21 (7%)	2 (1%)	22	60
21	cp	290/378 (77%)	263 (91%)	24 (8%)	3 (1%)	15	52
21	cq	280/378 (74%)	257 (92%)	21 (8%)	2 (1%)	22	60
21	cr	290/378 (77%)	264 (91%)	25 (9%)	1 (0%)	41	74
21	cs	273/378 (72%)	248 (91%)	23 (8%)	2 (1%)	22	60
21	ct	290/378 (77%)	258 (89%)	30 (10%)	2 (1%)	22	60
21	cu	278/378 (74%)	260 (94%)	18 (6%)	0	100	100
21	cv	290/378 (77%)	254 (88%)	34 (12%)	2 (1%)	22	60
21	cw	278/378 (74%)	252 (91%)	22 (8%)	4 (1%)	11	46
21	cx	290/378 (77%)	260 (90%)	30 (10%)	0	100	100
21	cy	278/378 (74%)	248 (89%)	29 (10%)	1 (0%)	34	70
21	cz	290/378 (77%)	267 (92%)	21 (7%)	2 (1%)	22	60
22	cO	28/1335 (2%)	21 (75%)	7 (25%)	0	100	100
22	cQ	29/1335 (2%)	22 (76%)	7 (24%)	0	100	100
22	da	30/1335 (2%)	24 (80%)	6 (20%)	0	100	100
22	dc	26/1335 (2%)	21 (81%)	5 (19%)	0	100	100
22	dg	30/1335 (2%)	27 (90%)	3 (10%)	0	100	100
22	di	27/1335 (2%)	21 (78%)	6 (22%)	0	100	100
22	ds	30/1335 (2%)	30 (100%)	0	0	100	100
22	du	28/1335 (2%)	24 (86%)	4 (14%)	0	100	100
23	cP	33/1369 (2%)	22 (67%)	11 (33%)	0	100	100
23	db	28/1369 (2%)	20 (71%)	6 (21%)	2 (7%)	1	17
23	dh	33/1369 (2%)	26 (79%)	7 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	dt	33/1369 (2%)	25 (76%)	8 (24%)	0	100	100
24	cR	397/400 (99%)	358 (90%)	34 (9%)	5 (1%)	12	48
24	cS	397/400 (99%)	359 (90%)	34 (9%)	4 (1%)	15	52
24	cT	397/400 (99%)	358 (90%)	35 (9%)	4 (1%)	15	52
25	cU	41/1343 (3%)	36 (88%)	5 (12%)	0	100	100
25	cV	41/1343 (3%)	35 (85%)	5 (12%)	1 (2%)	6	37
25	cW	41/1343 (3%)	36 (88%)	5 (12%)	0	100	100
26	dm	23/1359 (2%)	19 (83%)	4 (17%)	0	100	100
26	dn	23/1359 (2%)	18 (78%)	5 (22%)	0	100	100
26	do	23/1359 (2%)	21 (91%)	2 (9%)	0	100	100
All	All	54281/83744 (65%)	51687 (95%)	2389 (4%)	205 (0%)	38	70

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	ah	123	ASN
1	aU	123	ASN
1	bm	123	ASN
1	bo	123	ASN
1	br	123	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	aB	357/358 (100%)	357 (100%)	0	100	100
1	aC	357/358 (100%)	357 (100%)	0	100	100
1	aD	356/358 (99%)	355 (100%)	1 (0%)	92	96
1	aE	357/358 (100%)	357 (100%)	0	100	100
1	aF	356/358 (99%)	356 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aG	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	aH	356/358 (99%)	355 (100%)	1 (0%)	92	96
1	aI	357/358 (100%)	357 (100%)	0	100	100
1	aJ	357/358 (100%)	357 (100%)	0	100	100
1	aK	357/358 (100%)	357 (100%)	0	100	100
1	aL	356/358 (99%)	356 (100%)	0	100	100
1	aM	357/358 (100%)	357 (100%)	0	100	100
1	aN	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	aO	357/358 (100%)	357 (100%)	0	100	100
1	aP	357/358 (100%)	357 (100%)	0	100	100
1	aQ	356/358 (99%)	356 (100%)	0	100	100
1	aR	357/358 (100%)	357 (100%)	0	100	100
1	aS	357/358 (100%)	357 (100%)	0	100	100
1	aT	357/358 (100%)	357 (100%)	0	100	100
1	aU	357/358 (100%)	357 (100%)	0	100	100
1	aV	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	aW	357/358 (100%)	357 (100%)	0	100	100
1	aX	357/358 (100%)	357 (100%)	0	100	100
1	aY	357/358 (100%)	357 (100%)	0	100	100
1	aZ	357/358 (100%)	357 (100%)	0	100	100
1	aa	356/358 (99%)	356 (100%)	0	100	100
1	ab	357/358 (100%)	354 (99%)	3 (1%)	81	89
1	ac	357/358 (100%)	357 (100%)	0	100	100
1	ad	357/358 (100%)	357 (100%)	0	100	100
1	ae	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	af	357/358 (100%)	357 (100%)	0	100	100
1	ag	357/358 (100%)	357 (100%)	0	100	100
1	ah	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	ai	357/358 (100%)	357 (100%)	0	100	100
1	aj	357/358 (100%)	357 (100%)	0	100	100
1	ak	357/358 (100%)	356 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	al	356/358 (99%)	356 (100%)	0	100	100
1	am	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	an	356/358 (99%)	355 (100%)	1 (0%)	92	96
1	ao	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	ap	357/358 (100%)	357 (100%)	0	100	100
1	aq	357/358 (100%)	357 (100%)	0	100	100
1	ar	356/358 (99%)	356 (100%)	0	100	100
1	as	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	at	357/358 (100%)	357 (100%)	0	100	100
1	au	356/358 (99%)	356 (100%)	0	100	100
1	av	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	aw	357/358 (100%)	357 (100%)	0	100	100
1	ax	356/358 (99%)	356 (100%)	0	100	100
1	ay	357/358 (100%)	357 (100%)	0	100	100
1	az	356/358 (99%)	356 (100%)	0	100	100
1	ba	357/358 (100%)	357 (100%)	0	100	100
1	bb	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	bc	357/358 (100%)	357 (100%)	0	100	100
1	bd	357/358 (100%)	357 (100%)	0	100	100
1	be	357/358 (100%)	357 (100%)	0	100	100
1	bf	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	bg	357/358 (100%)	357 (100%)	0	100	100
1	bh	357/358 (100%)	357 (100%)	0	100	100
1	bi	357/358 (100%)	357 (100%)	0	100	100
1	bj	357/358 (100%)	357 (100%)	0	100	100
1	bk	357/358 (100%)	355 (99%)	2 (1%)	86	92
1	bl	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	bm	357/358 (100%)	357 (100%)	0	100	100
1	bn	356/358 (99%)	356 (100%)	0	100	100
1	bo	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	bp	357/358 (100%)	357 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	bq	357/358 (100%)	357 (100%)	0	100	100
1	br	357/358 (100%)	356 (100%)	1 (0%)	92	96
1	bs	357/358 (100%)	357 (100%)	0	100	100
1	bt	357/358 (100%)	357 (100%)	0	100	100
2	bA	438/441 (99%)	435 (99%)	3 (1%)	84	91
2	bB	439/441 (100%)	439 (100%)	0	100	100
2	bu	439/441 (100%)	434 (99%)	5 (1%)	73	85
2	bv	439/441 (100%)	434 (99%)	5 (1%)	73	85
2	bw	439/441 (100%)	438 (100%)	1 (0%)	93	97
2	bx	438/441 (99%)	435 (99%)	3 (1%)	84	91
2	by	439/441 (100%)	438 (100%)	1 (0%)	93	97
2	bz	432/441 (98%)	429 (99%)	3 (1%)	84	91
3	bC	439/440 (100%)	439 (100%)	0	100	100
4	bD	344/346 (99%)	343 (100%)	1 (0%)	92	96
4	bF	344/346 (99%)	343 (100%)	1 (0%)	92	96
4	cX	343/346 (99%)	341 (99%)	2 (1%)	86	92
4	cZ	343/346 (99%)	343 (100%)	0	100	100
4	dd	344/346 (99%)	343 (100%)	1 (0%)	92	96
4	df	343/346 (99%)	342 (100%)	1 (0%)	92	96
4	dj	344/346 (99%)	342 (99%)	2 (1%)	86	92
4	dk	344/346 (99%)	340 (99%)	4 (1%)	71	84
4	dl	344/346 (99%)	343 (100%)	1 (0%)	92	96
4	dp	344/346 (99%)	344 (100%)	0	100	100
4	dr	344/346 (99%)	344 (100%)	0	100	100
5	bE	349/353 (99%)	348 (100%)	1 (0%)	92	96
5	cY	349/353 (99%)	347 (99%)	2 (1%)	86	92
5	de	349/353 (99%)	348 (100%)	1 (0%)	92	96
5	dq	349/353 (99%)	348 (100%)	1 (0%)	92	96
6	bG	424/446 (95%)	424 (100%)	0	100	100
7	bH	345/479 (72%)	345 (100%)	0	100	100
8	bI	116/144 (81%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	bJ	122/144 (85%)	122 (100%)	0	100	100
8	bK	93/144 (65%)	93 (100%)	0	100	100
9	bL	59/161 (37%)	59 (100%)	0	100	100
9	bM	59/161 (37%)	58 (98%)	1 (2%)	60	78
9	bN	58/161 (36%)	58 (100%)	0	100	100
9	bO	58/161 (36%)	57 (98%)	1 (2%)	60	78
10	bP	121/125 (97%)	121 (100%)	0	100	100
11	bQ	140/188 (74%)	139 (99%)	1 (1%)	84	91
12	bR	136/148 (92%)	136 (100%)	0	100	100
13	bS	164/179 (92%)	164 (100%)	0	100	100
14	bT	40/181 (22%)	40 (100%)	0	100	100
14	bU	47/181 (26%)	47 (100%)	0	100	100
14	bV	46/181 (25%)	46 (100%)	0	100	100
14	bW	45/181 (25%)	45 (100%)	0	100	100
14	bX	35/181 (19%)	35 (100%)	0	100	100
14	bY	62/181 (34%)	62 (100%)	0	100	100
14	bZ	45/181 (25%)	45 (100%)	0	100	100
14	ca	45/181 (25%)	44 (98%)	1 (2%)	52	72
14	cb	45/181 (25%)	45 (100%)	0	100	100
14	cc	72/181 (40%)	71 (99%)	1 (1%)	67	81
14	cd	63/181 (35%)	62 (98%)	1 (2%)	62	79
14	ce	60/181 (33%)	60 (100%)	0	100	100
15	cf	70/139 (50%)	70 (100%)	0	100	100
16	cg	51/79 (65%)	51 (100%)	0	100	100
17	ch	142/145 (98%)	141 (99%)	1 (1%)	84	91
18	ci	47/63 (75%)	47 (100%)	0	100	100
19	cj	51/70 (73%)	51 (100%)	0	100	100
19	ck	49/70 (70%)	49 (100%)	0	100	100
19	cl	47/70 (67%)	47 (100%)	0	100	100
19	cm	54/70 (77%)	54 (100%)	0	100	100
20	cn	84/130 (65%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	co	78/130 (60%)	78 (100%)	0	100	100
21	cA	245/339 (72%)	244 (100%)	1 (0%)	91	95
21	cB	257/339 (76%)	256 (100%)	1 (0%)	91	95
21	cC	245/339 (72%)	244 (100%)	1 (0%)	91	95
21	cD	257/339 (76%)	257 (100%)	0	100	100
21	cE	246/339 (73%)	245 (100%)	1 (0%)	91	95
21	cF	257/339 (76%)	255 (99%)	2 (1%)	81	89
21	cG	248/339 (73%)	246 (99%)	2 (1%)	81	89
21	cH	257/339 (76%)	257 (100%)	0	100	100
21	cI	245/339 (72%)	244 (100%)	1 (0%)	91	95
21	cJ	257/339 (76%)	256 (100%)	1 (0%)	91	95
21	cK	245/339 (72%)	244 (100%)	1 (0%)	91	95
21	cL	257/339 (76%)	257 (100%)	0	100	100
21	cM	243/339 (72%)	242 (100%)	1 (0%)	91	95
21	cN	257/339 (76%)	256 (100%)	1 (0%)	91	95
21	cp	257/339 (76%)	257 (100%)	0	100	100
21	cq	248/339 (73%)	248 (100%)	0	100	100
21	cr	257/339 (76%)	257 (100%)	0	100	100
21	cs	241/339 (71%)	240 (100%)	1 (0%)	91	95
21	ct	257/339 (76%)	257 (100%)	0	100	100
21	cu	246/339 (73%)	246 (100%)	0	100	100
21	cv	257/339 (76%)	257 (100%)	0	100	100
21	cw	246/339 (73%)	246 (100%)	0	100	100
21	cx	257/339 (76%)	256 (100%)	1 (0%)	91	95
21	cy	246/339 (73%)	246 (100%)	0	100	100
21	cz	257/339 (76%)	257 (100%)	0	100	100
22	cO	22/1123 (2%)	22 (100%)	0	100	100
22	cQ	25/1123 (2%)	24 (96%)	1 (4%)	31	59
22	da	24/1123 (2%)	24 (100%)	0	100	100
22	dc	22/1123 (2%)	22 (100%)	0	100	100
22	dg	26/1123 (2%)	25 (96%)	1 (4%)	33	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	di	22/1123 (2%)	22 (100%)	0	100	100
22	ds	25/1123 (2%)	25 (100%)	0	100	100
22	du	24/1123 (2%)	24 (100%)	0	100	100
23	cP	24/1147 (2%)	24 (100%)	0	100	100
23	db	19/1147 (2%)	19 (100%)	0	100	100
23	dh	26/1147 (2%)	25 (96%)	1 (4%)	33	61
23	dt	24/1147 (2%)	24 (100%)	0	100	100
24	cR	359/360 (100%)	358 (100%)	1 (0%)	92	96
24	cS	359/360 (100%)	358 (100%)	1 (0%)	92	96
24	cT	359/360 (100%)	359 (100%)	0	100	100
25	cU	30/1015 (3%)	30 (100%)	0	100	100
25	cV	28/1015 (3%)	28 (100%)	0	100	100
25	cW	29/1015 (3%)	29 (100%)	0	100	100
26	dm	17/1144 (2%)	17 (100%)	0	100	100
26	dn	19/1144 (2%)	19 (100%)	0	100	100
26	do	19/1144 (2%)	18 (95%)	1 (5%)	22	54
All	All	45770/70345 (65%)	45679 (100%)	91 (0%)	93	97

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	cA	289	LYS
24	cR	295	ARG
21	cC	277	ARG
21	cI	277	ARG
5	cY	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
1	bm	187	ASN
22	dg	37	GLN
2	bB	483	GLN
4	df	275	ASN
21	cN	333	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

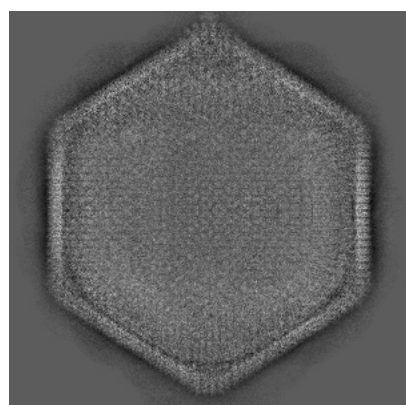
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34438. These allow visual inspection of the internal detail of the map and identification of artifacts.

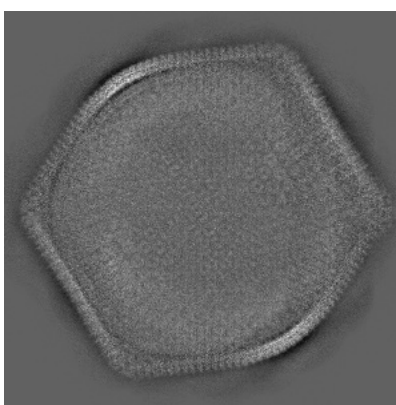
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

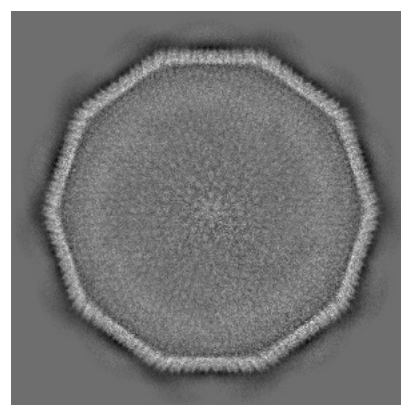
6.1.1 Primary map



X



Y

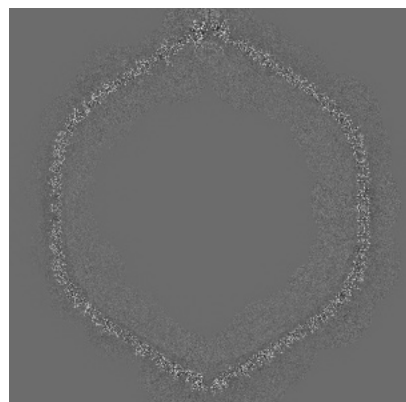


Z

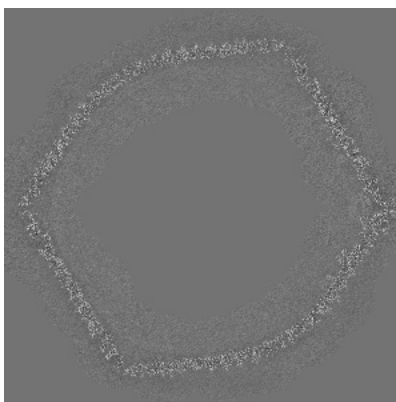
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

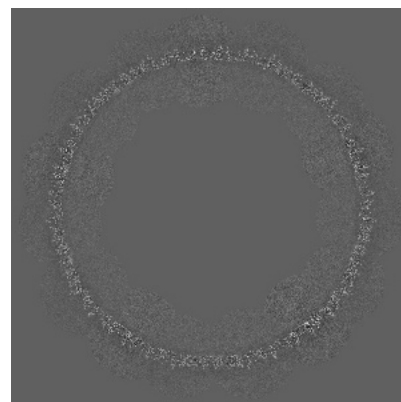
6.2.1 Primary map



X Index: 600



Y Index: 600

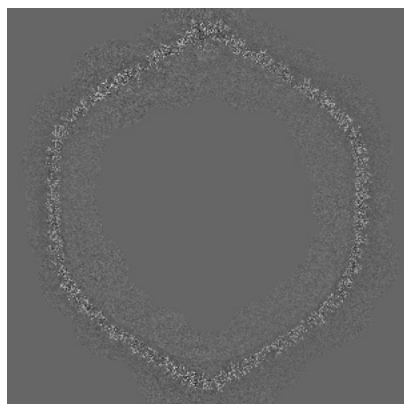


Z Index: 600

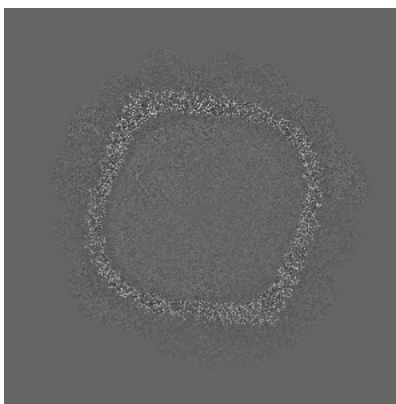
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

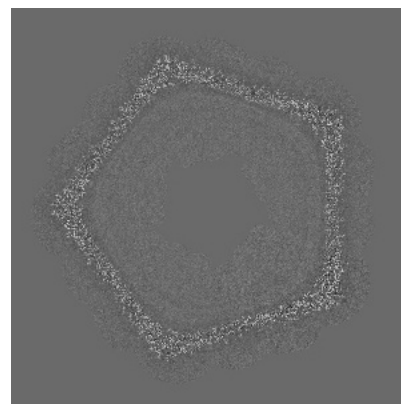
6.3.1 Primary map



X Index: 628



Y Index: 257



Z Index: 320

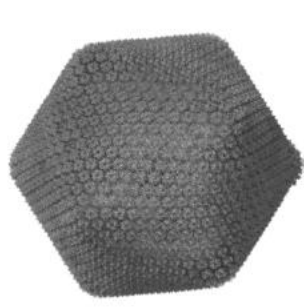
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

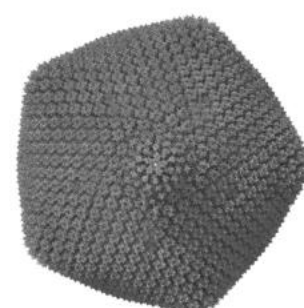
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

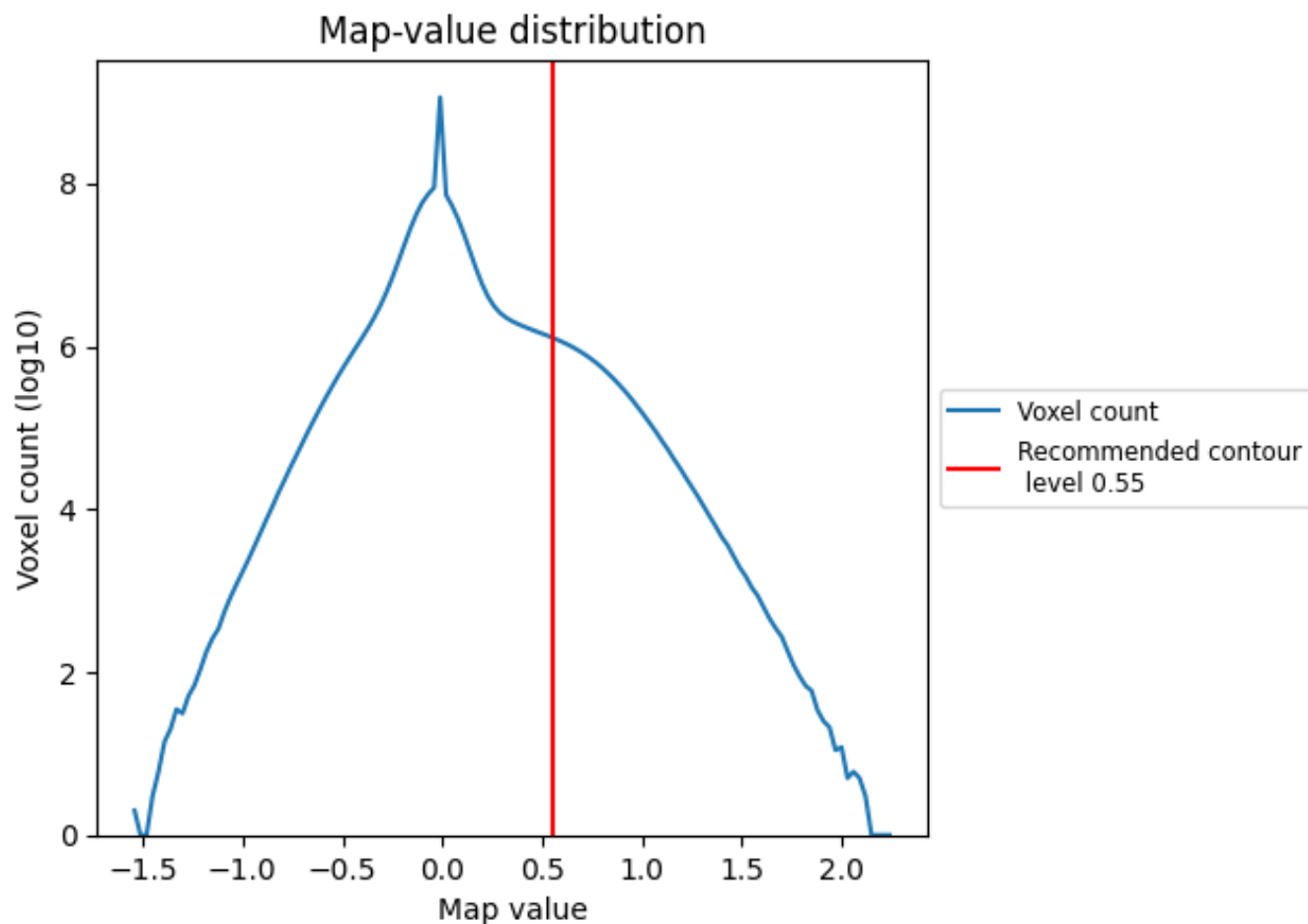
6.5 Mask visualisation

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

7 Map analysis [i](#)

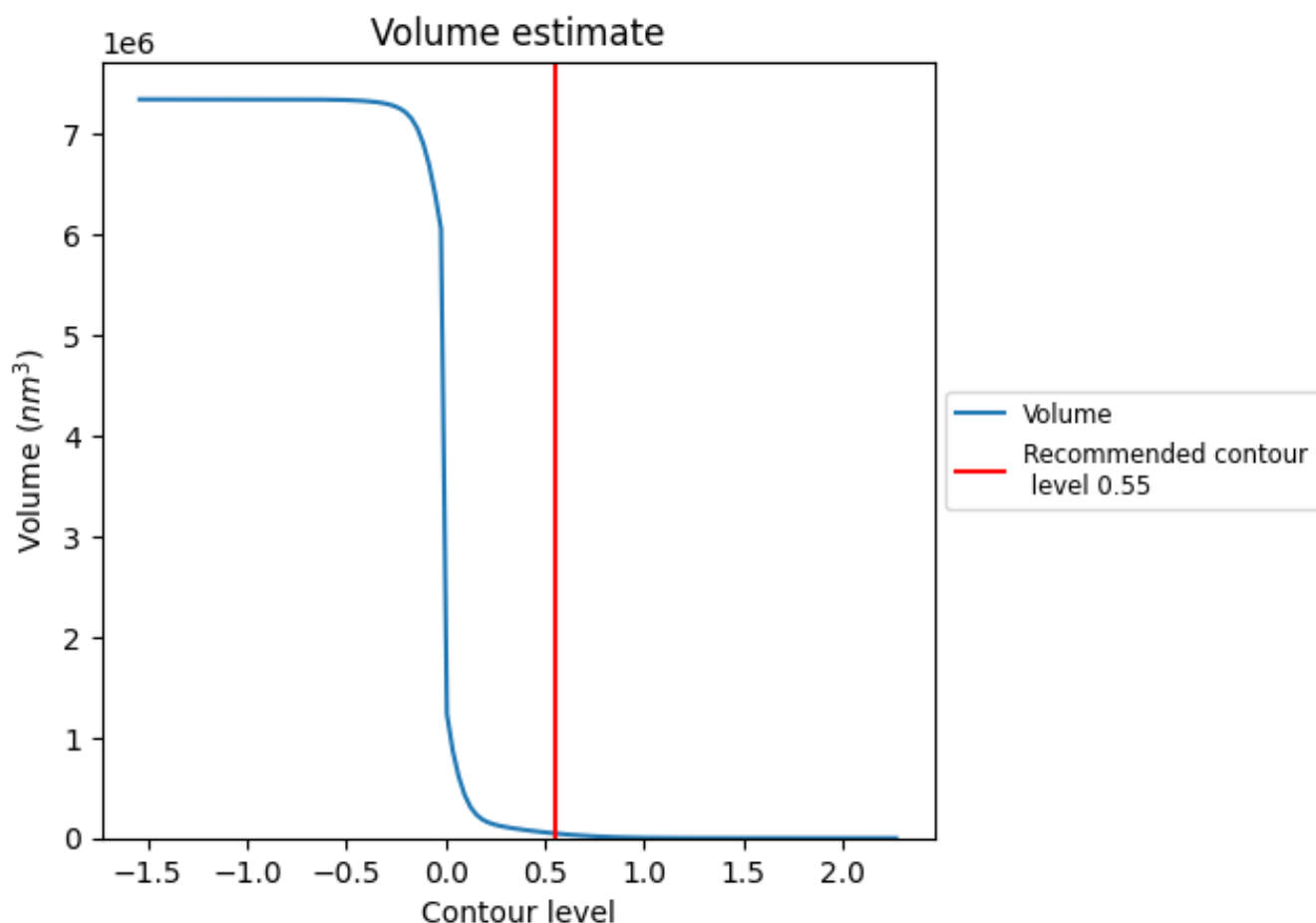
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

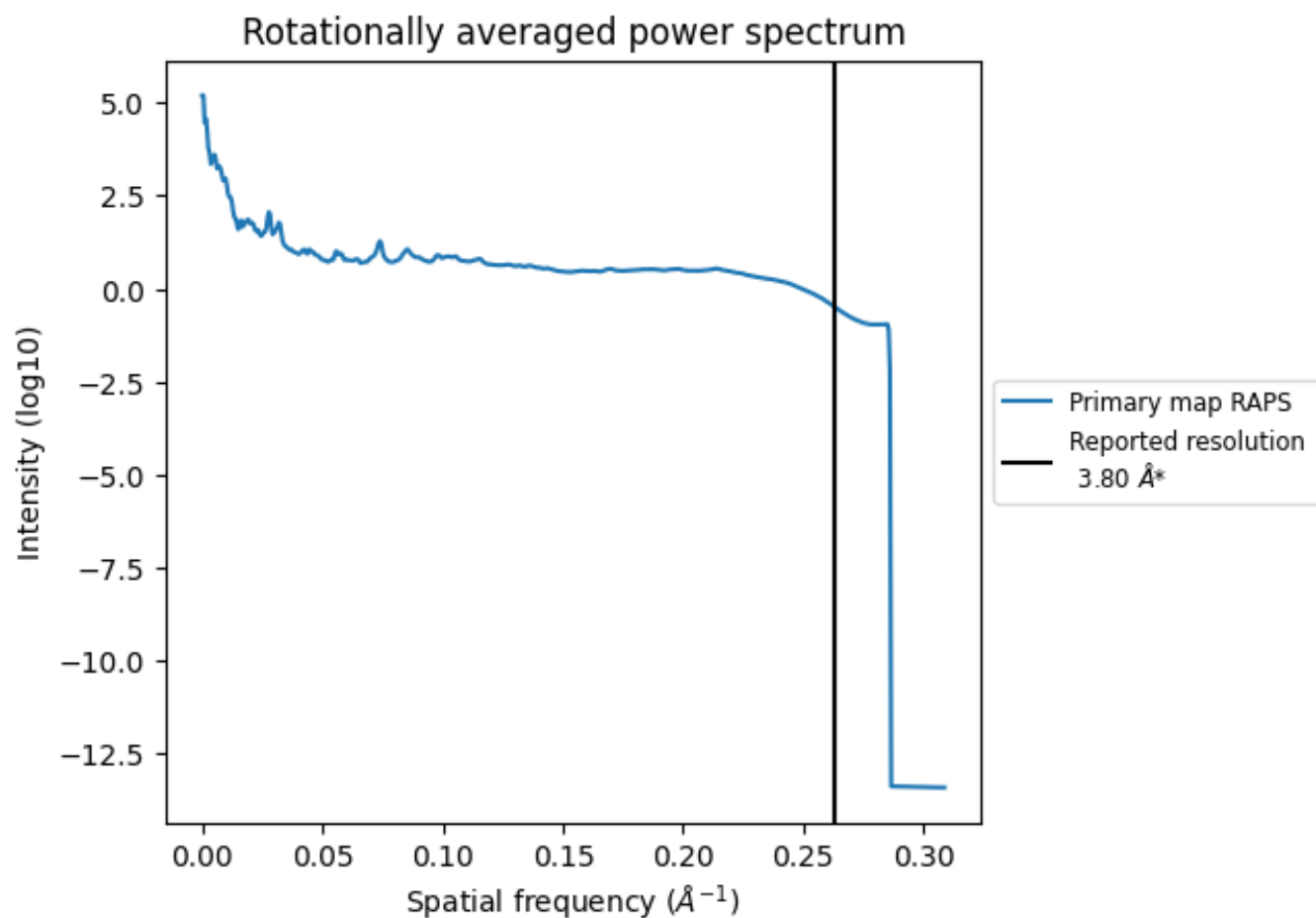
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46843 nm³; this corresponds to an approximate mass of 42315 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 0.263 Å⁻¹

8 Fourier-Shell correlation

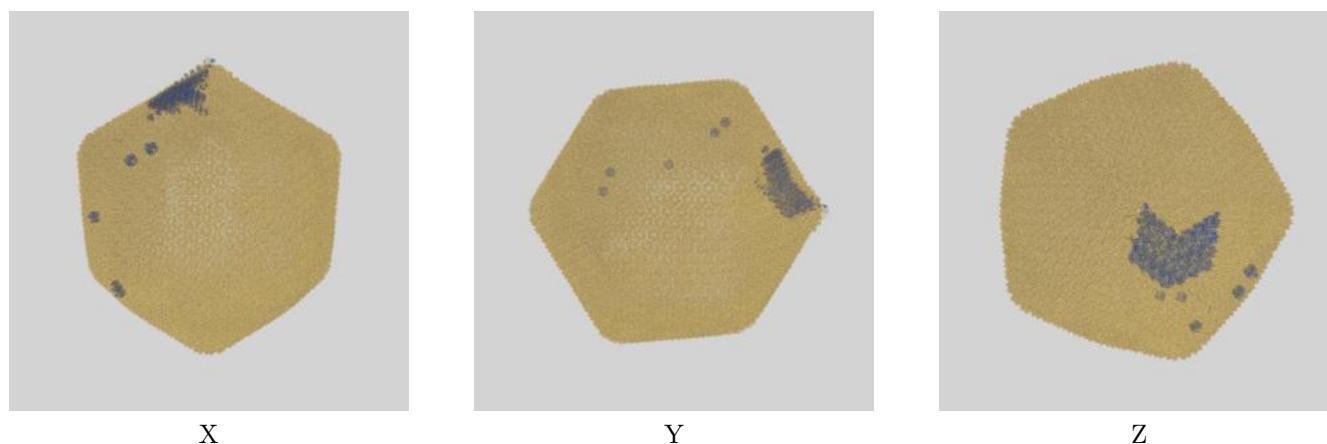
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

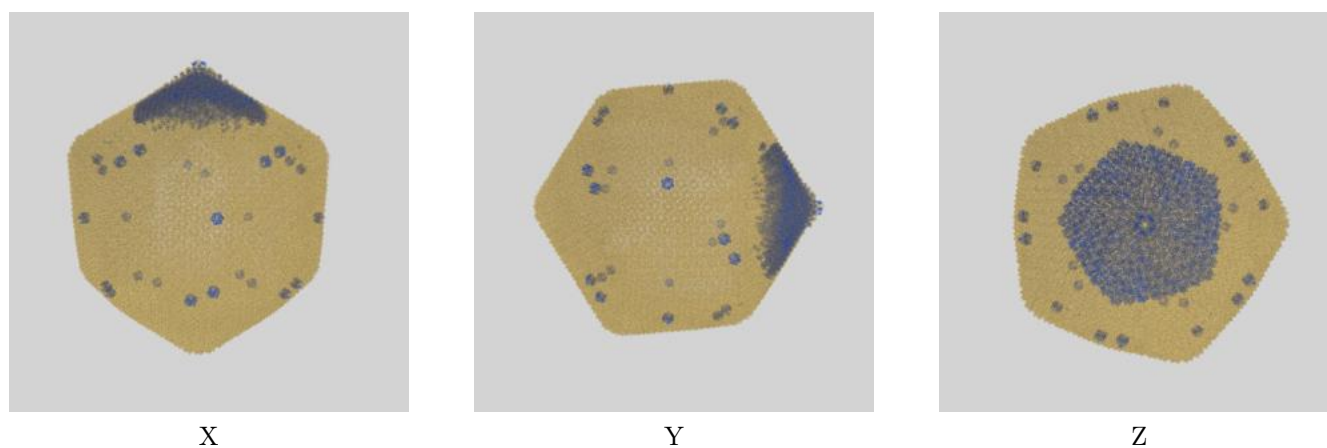
This section contains information regarding the fit between EMDB map EMD-34438 and PDB model 8H2I. Per-residue inclusion information can be found in section 3 on page 22.

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 0.55 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](#)



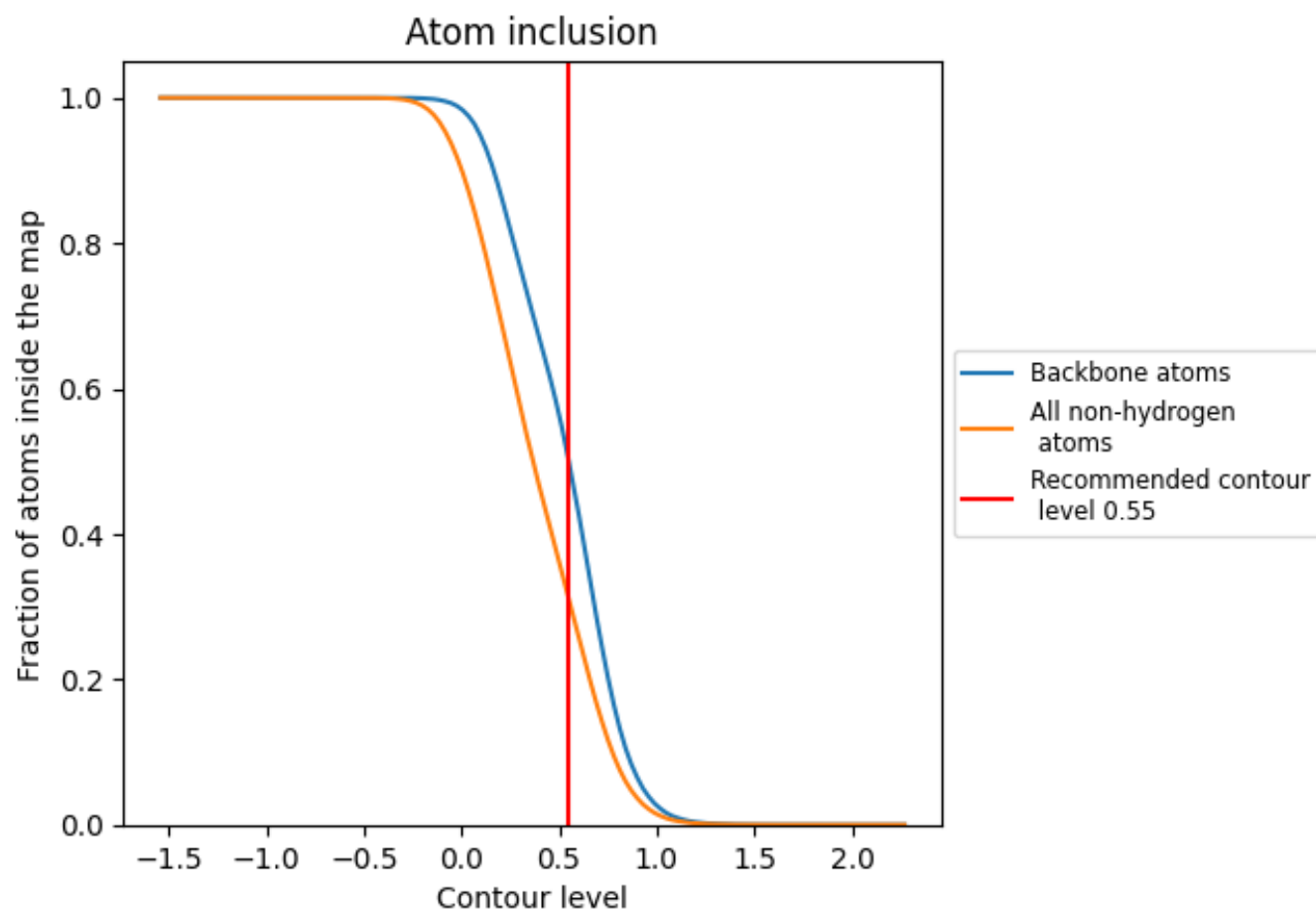
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 31% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3109	 0.3620
aA	 0.2584	 0.3860
aB	 0.2671	 0.3810
aC	 0.2862	 0.3790
aD	 0.2937	 0.3800
aE	 0.3827	 0.4000
aF	 0.4162	 0.3950
aG	 0.3707	 0.3900
aH	 0.4419	 0.4010
aI	 0.4387	 0.4000
aJ	 0.4140	 0.3930
aK	 0.3897	 0.3960
aL	 0.3659	 0.3930
aM	 0.3608	 0.3940
aN	 0.3692	 0.3970
aO	 0.3656	 0.3900
aP	 0.3749	 0.3960
aQ	 0.3369	 0.3910
aR	 0.3307	 0.3900
aS	 0.3506	 0.3970
aT	 0.3662	 0.3910
aU	 0.3800	 0.3960
aV	 0.3800	 0.3970
aW	 0.3310	 0.3900
aX	 0.3339	 0.3900
aY	 0.3316	 0.3900
aZ	 0.3521	 0.3910
aa	 0.4215	 0.3970
ab	 0.4248	 0.3940
ac	 0.4330	 0.4050
ad	 0.4336	 0.3980
ae	 0.4251	 0.4010
af	 0.4218	 0.4010
ag	 0.4155	 0.3910
ah	 0.4504	 0.4050























































































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Chain	Atom inclusion	Q-score
ai	 0.4230	 0.3990
aj	 0.3016	 0.3830
ak	 0.3608	 0.3940
al	 0.2939	 0.3800
am	 0.4336	 0.3980
an	 0.4370	 0.3950
ao	 0.4258	 0.3960
ap	 0.4429	 0.3980
aq	 0.4621	 0.3980
ar	 0.4609	 0.4010
as	 0.4251	 0.3900
at	 0.3845	 0.3990
au	 0.3933	 0.4020
av	 0.3319	 0.3890
aw	 0.3031	 0.3940
ax	 0.3480	 0.3980
ay	 0.2328	 0.3780
az	 0.2219	 0.3830
bA	 0.3616	 0.3680
bB	 0.2714	 0.3590
bC	 0.3452	 0.3730
bD	 0.2304	 0.3510
bE	 0.2899	 0.3580
bF	 0.2638	 0.3460
bG	 0.3264	 0.3190
bH	 0.3214	 0.3860
bI	 0.3007	 0.3470
bJ	 0.3125	 0.3430
bK	 0.3061	 0.3660
bL	 0.2548	 0.2560
bM	 0.2375	 0.2780
bN	 0.2583	 0.2770
bO	 0.2133	 0.2690
bP	 0.2445	 0.3230
bQ	 0.2139	 0.3340
bR	 0.3369	 0.3500
bS	 0.3116	 0.3890
bT	 0.3152	 0.3600
bU	 0.4402	 0.3720
bV	 0.3780	 0.3510
bW	 0.3784	 0.3380
bX	 0.3420	 0.3510





















































































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Chain	Atom inclusion	Q-score
bY	 0.2228	 0.3100
bZ	 0.1955	 0.3360
ba	 0.3785	 0.3920
bb	 0.3443	 0.3980
bc	 0.3710	 0.3880
bd	 0.3590	 0.3920
be	 0.3650	 0.3910
bf	 0.3857	 0.3930
bg	 0.3704	 0.3880
bh	 0.3879	 0.3900
bi	 0.3692	 0.3950
bj	 0.3394	 0.3920
bk	 0.3722	 0.3900
bl	 0.3488	 0.3960
bm	 0.3400	 0.3930
bn	 0.3353	 0.4010
bo	 0.3388	 0.3910
bp	 0.3671	 0.3890
bq	 0.3352	 0.3870
br	 0.3990	 0.3920
bs	 0.3731	 0.3880
bt	 0.3839	 0.3930
bu	 0.4828	 0.3820
bv	 0.4510	 0.3760
bw	 0.4613	 0.3780
bx	 0.4272	 0.3790
by	 0.4070	 0.3760
bz	 0.4051	 0.3700
cA	 0.0000	 0.1280
cB	 0.0591	 0.2680
cC	 0.0014	 0.2080
cD	 0.0216	 0.2300
cE	 0.0378	 0.2070
cF	 0.1186	 0.2600
cG	 0.0270	 0.1770
cH	 0.2275	 0.2810
cI	 0.0088	 0.2100
cJ	 0.1477	 0.2890
cK	 0.0005	 0.1880
cL	 0.0802	 0.2810
cM	 0.0000	 0.1290
cN	 0.0110	 0.2370



































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Chain	Atom inclusion	Q-score
cO	 0.0000	 0.4580
cP	 0.0084	 0.4540
cQ	 0.0131	 0.4490
cR	 0.2879	 0.3690
cS	 0.3092	 0.3610
cT	 0.2752	 0.3470
cU	 0.1424	 0.4210
cV	 0.1584	 0.4140
cW	 0.1699	 0.4200
cX	 0.3112	 0.3360
cY	 0.2553	 0.3320
cZ	 0.3025	 0.3400
ca	 0.2256	 0.3680
cb	 0.2456	 0.3550
cc	 0.2609	 0.3240
cd	 0.2652	 0.3370
ce	 0.3123	 0.3590
cf	 0.3639	 0.3430
cg	 0.1614	 0.3070
ch	 0.3601	 0.3560
ci	 0.4022	 0.3530
cj	 0.2721	 0.3750
ck	 0.2081	 0.3810
cl	 0.2500	 0.3610
cm	 0.2690	 0.3710
cn	 0.2411	 0.3910
co	 0.2673	 0.3680
cp	 0.0238	 0.2540
cq	 0.0000	 0.1670
cr	 0.0613	 0.2610
cs	 0.0019	 0.1780
ct	 0.0516	 0.2710
cu	 0.0014	 0.1850
cv	 0.1609	 0.2950
cw	 0.1093	 0.2620
cx	 0.2125	 0.2930
cy	 0.0350	 0.2420
cz	 0.0110	 0.2100
da	 0.0881	 0.4680
db	 0.1106	 0.4280
dc	 0.1122	 0.4710
dd	 0.2413	 0.3720

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Chain	Atom inclusion	Q-score
de	 0.2252	 0.3630
df	 0.2394	 0.3680
dg	 0.0084	 0.4510
dh	 0.0081	 0.4250
di	 0.0000	 0.4400
dj	 0.2867	 0.3620
dk	 0.2661	 0.3550
dl	 0.2992	 0.3340
dm	 0.0000	 0.3540
dn	 0.0111	 0.3860
do	 0.0000	 0.3280
dp	 0.3012	 0.3750
dq	 0.2960	 0.3750
dr	 0.3089	 0.3720
ds	 0.0299	 0.4410
dt	 0.0171	 0.4570
du	 0.0045	 0.4400