Full wwPDB EM Validation 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

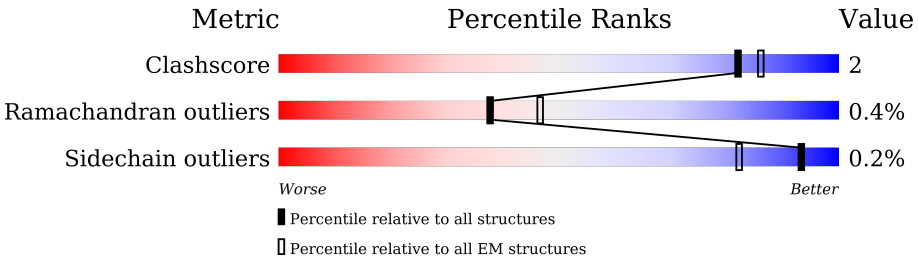
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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 <=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	85% 99%
1	aB	437	81% 100%
1	aC	437	78% 100%
1	aD	437	78% 99%
1	aE	437	52% 100%
1	aF	437	44% 99%
1	aG	437	59% 99%
1	aH	437	38% 99%

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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	61% 90% 9%
14	bT	207	16% 22% 77%
14	bU	207	12% 26% 74%
14	bV	207	14% 25% 74%
14	bW	207	14% 25% 75%
14	bX	207	13% 19% 80%
14	bY	207	29% 34% 64%
14	bZ	207	23% 25% 75%
14	ca	207	23% 24% 75%
14	cb	207	21% 25% 75%
14	cc	207	28% 40% 59%
14	cd	207	27% 36% 64%
14	ce	207	26% 34% 65%
15	cf	151	34% 50% 48%
16	cg	98	59% 64% 33%
17	ch	155	59% 96%
18	ci	93	40% 84% 14%
19	cj	80	54% 74% 26%
19	ck	80	55% 71% 29%
19	cl	80	52% 69% 31%
19	cm	80	54% 79% 21%
20	cn	148	54% 66% 34%
20	co	148	47% 64% 36%
21	cA	378	74% 74% 26%
21	cB	378	76% 77% 23%

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Mol	Chain	Length	Quality of chain
21	cC	378	74% 73% 26%
21	cD	378	77% 76% 23%
21	cE	378	73% 73% 26%
21	cF	378	74% 76% 23%
21	cG	378	74% 74% 25%
21	cH	378	63% 77% 23%
21	cI	378	74% 74% 26%
21	cJ	378	71% 76% 23%
21	cK	378	74% 73% 26%
21	cL	378	75% 77% 23%
21	cM	378	73% 73% 27%
21	cN	378	77% 76% 23%
21	cp	378	77% 76% 23%
21	cq	378	75% 74% 25%
21	cr	378	76% 77% 23%
21	cs	378	73% 72% 27%
21	ct	378	76% 77% 23%
21	cu	378	74% 74% 26%
21	cv	378	72% 77% 23%
21	cw	378	71% 73% 26%
21	cx	378	63% 77% 23%
21	cy	378	72% 74% 26%
21	cz	378	77% 77% 23%
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 (i)

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 211	C 137	N 32	O 40	S 2	0	0
22	ds	32	Total 238	C 152	N 40	O 44	S 2	0	0
22	du	30	Total 224	C 144	N 36	O 42	S 2	0	0

- Molecule 23 is a protein called P21.

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

- Molecule 24 is a protein called MCPv5.

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

- Molecule 25 is a protein called P22.

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

- Molecule 26 is a protein called P23.

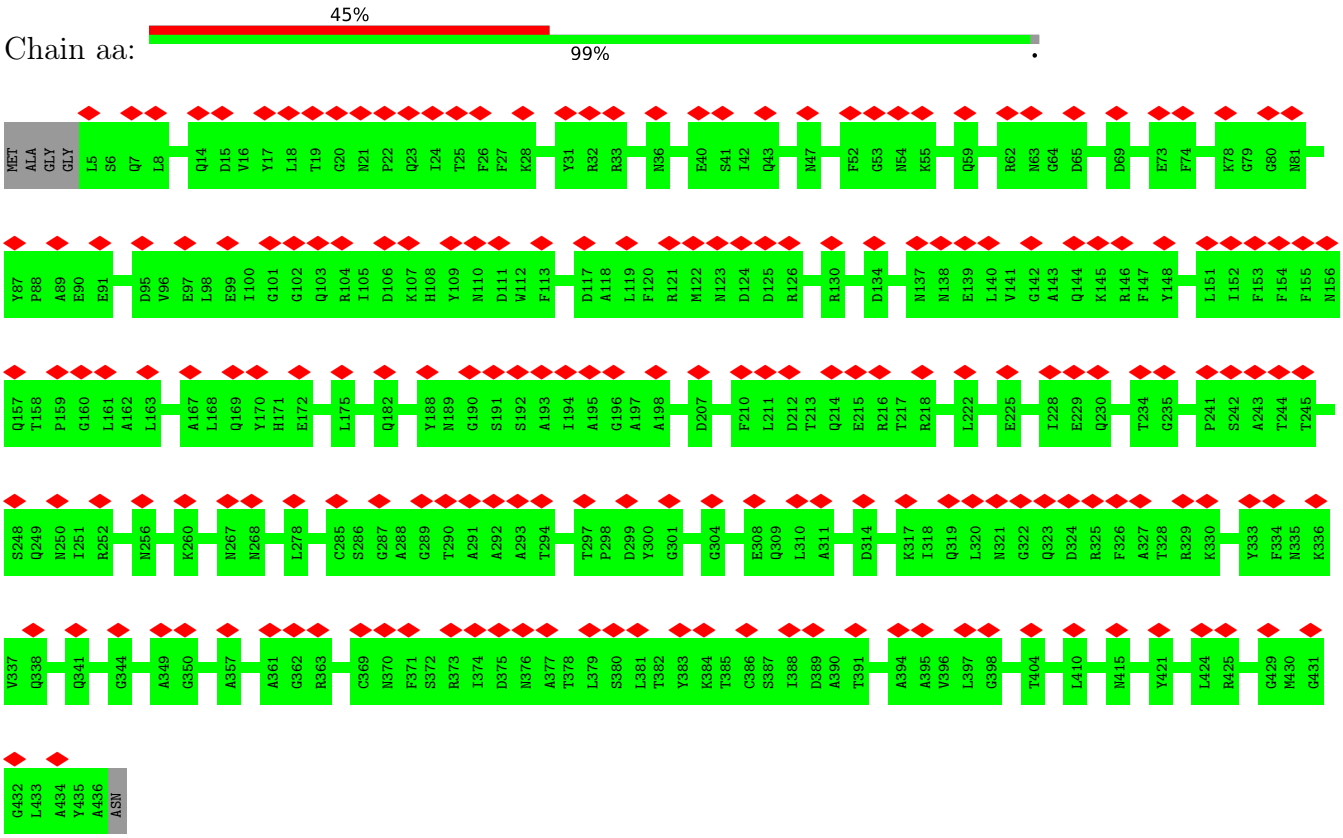
Mol	Chain	Residues	Atoms				AltConf	Trace
26	dm	25	Total	C	N	O	0	0
			174	111	28	35		
26	dn	25	Total	C	N	O	0	0
			181	116	29	36		
26	do	25	Total	C	N	O	0	0
			182	121	28	33		

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.

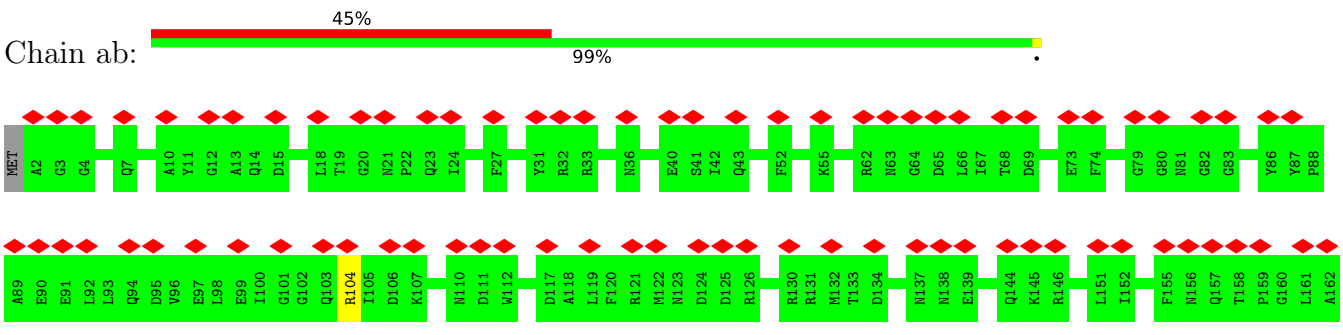
• Molecule 1: Major capsid protein (MCP)

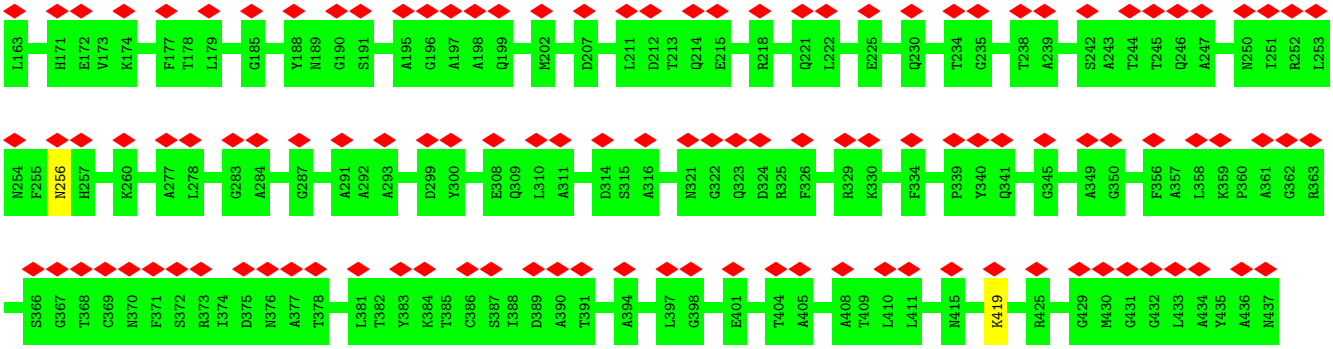
Chain aa:



• Molecule 1: Major capsid protein (MCP)

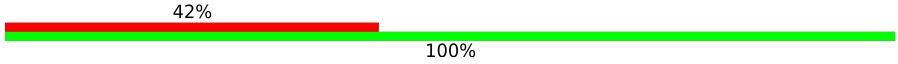
Chain ab:

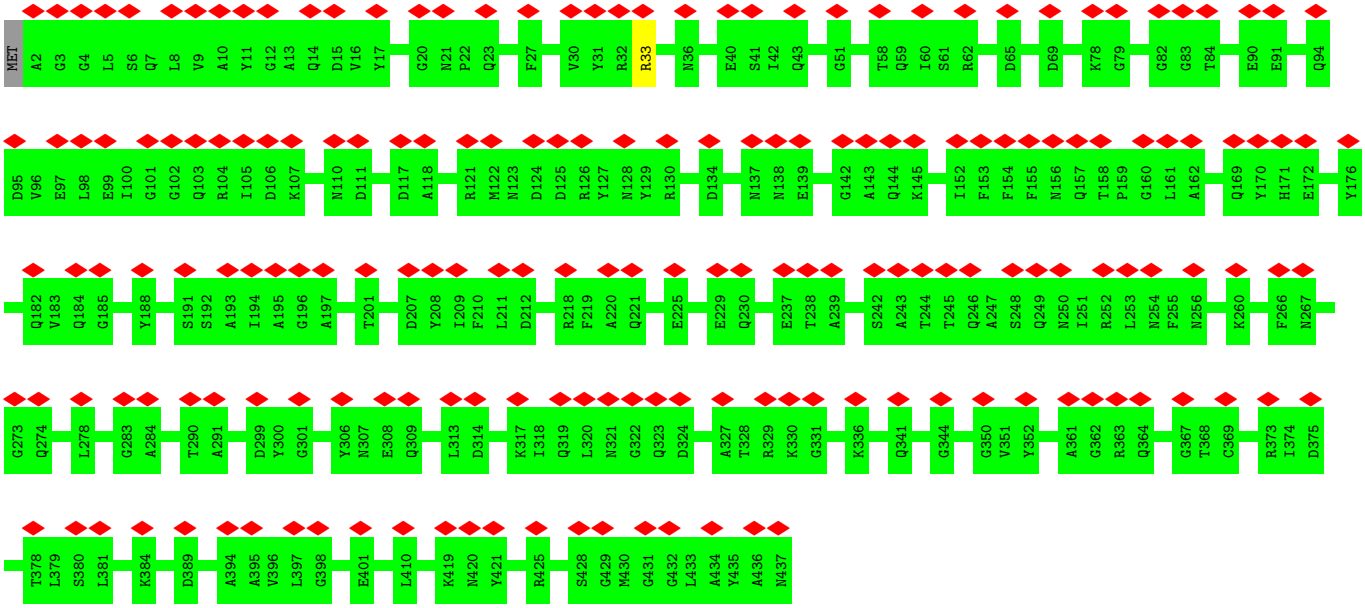




• Molecule 1: Major capsid protein (MCP)

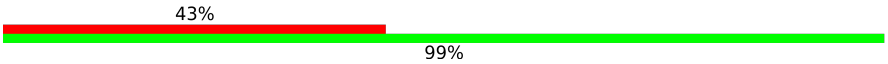
Chain ac:

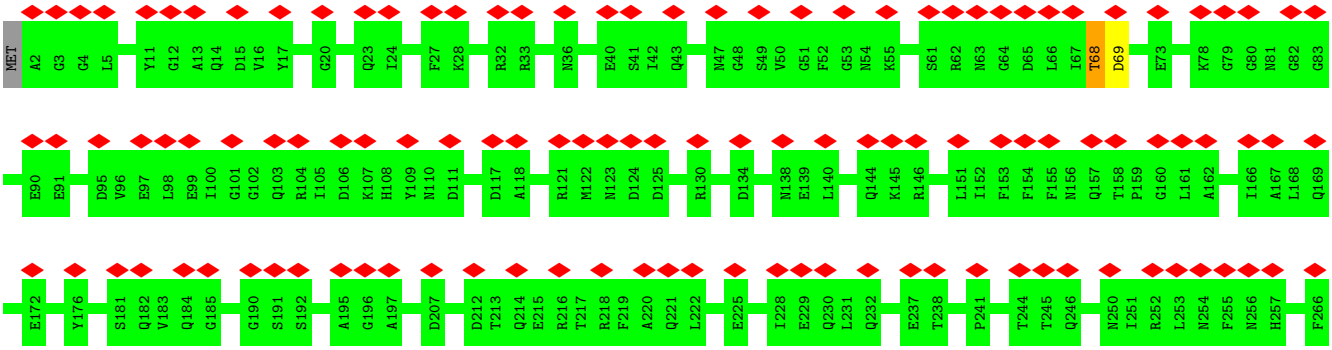


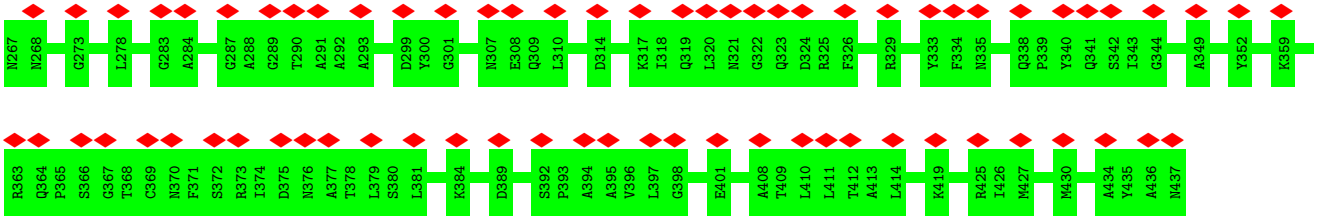


• Molecule 1: Major capsid protein (MCP)

Chain ad:

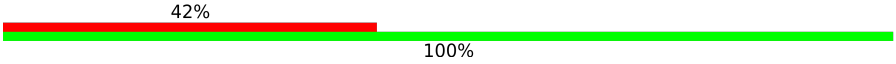


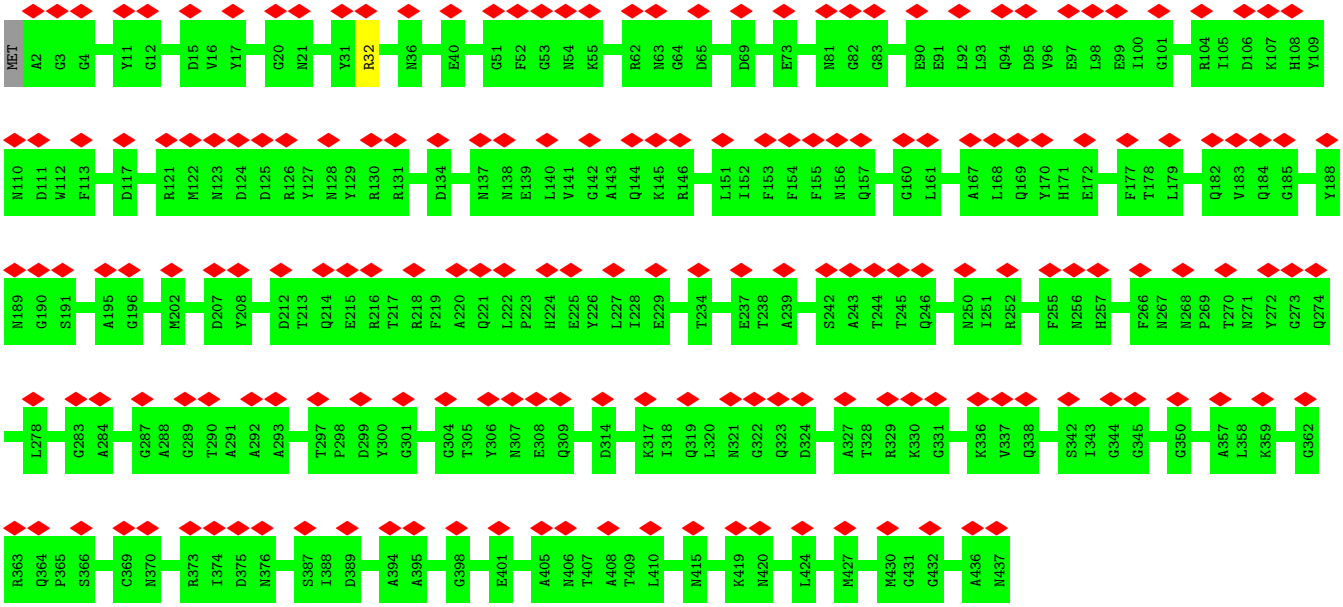




• Molecule 1: Major capsid protein (MCP)

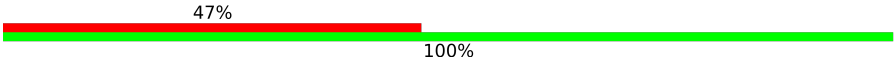
Chain ae:

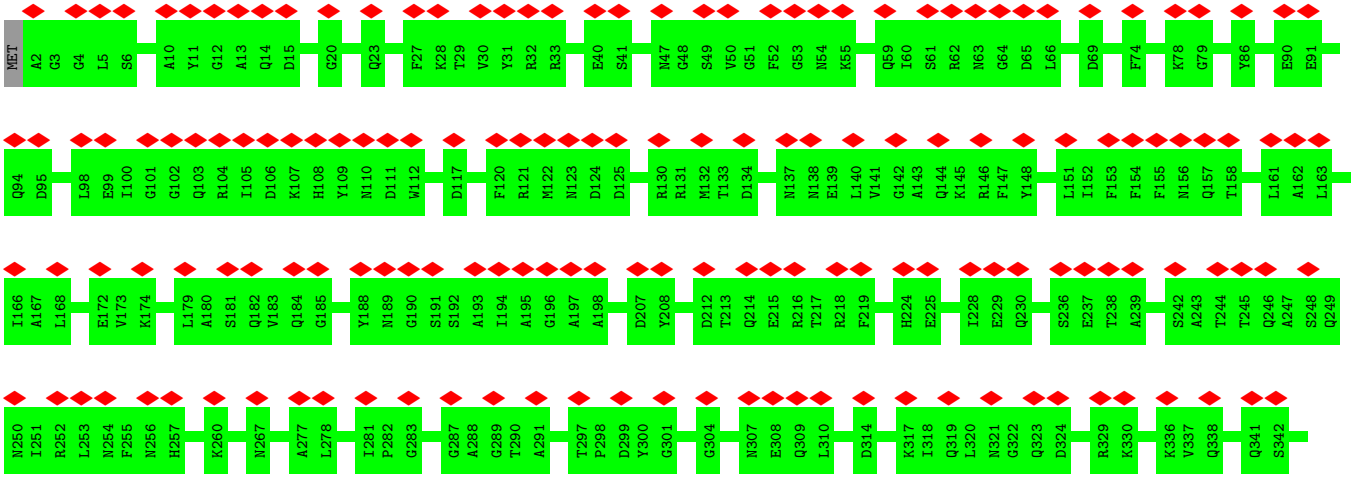


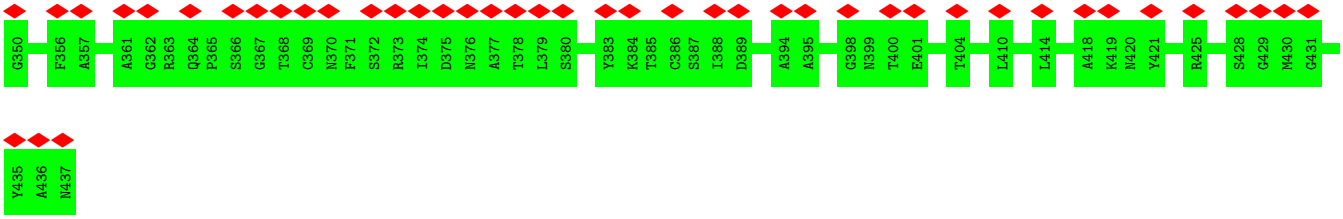


• Molecule 1: Major capsid protein (MCP)

Chain af:

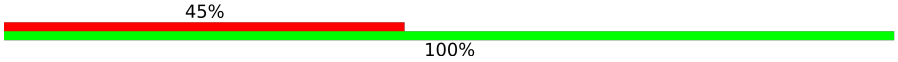






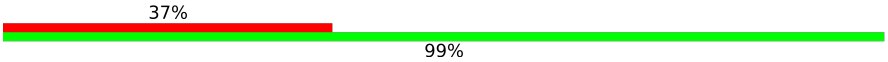
• Molecule 1: Major capsid protein (MCP)

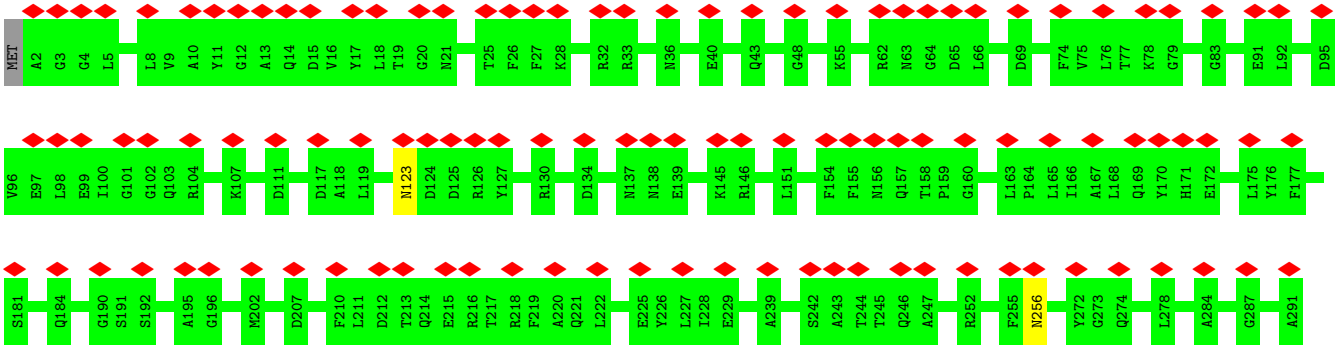
Chain ag:



• Molecule 1: Major capsid protein (MCP)

Chain ah:





• Molecule 1: Major capsid protein (MCP)

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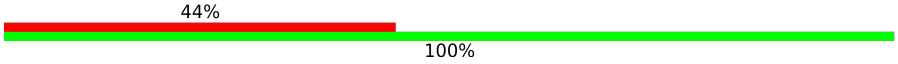

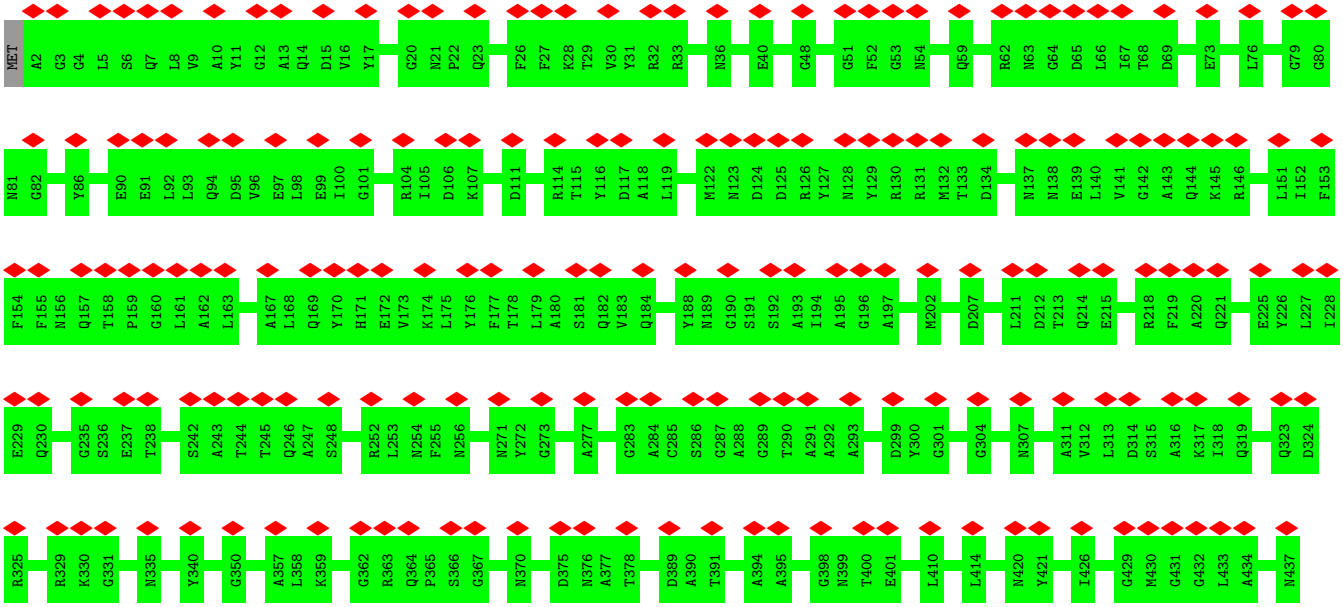

• Molecule 1: Major capsid protein (MCP)

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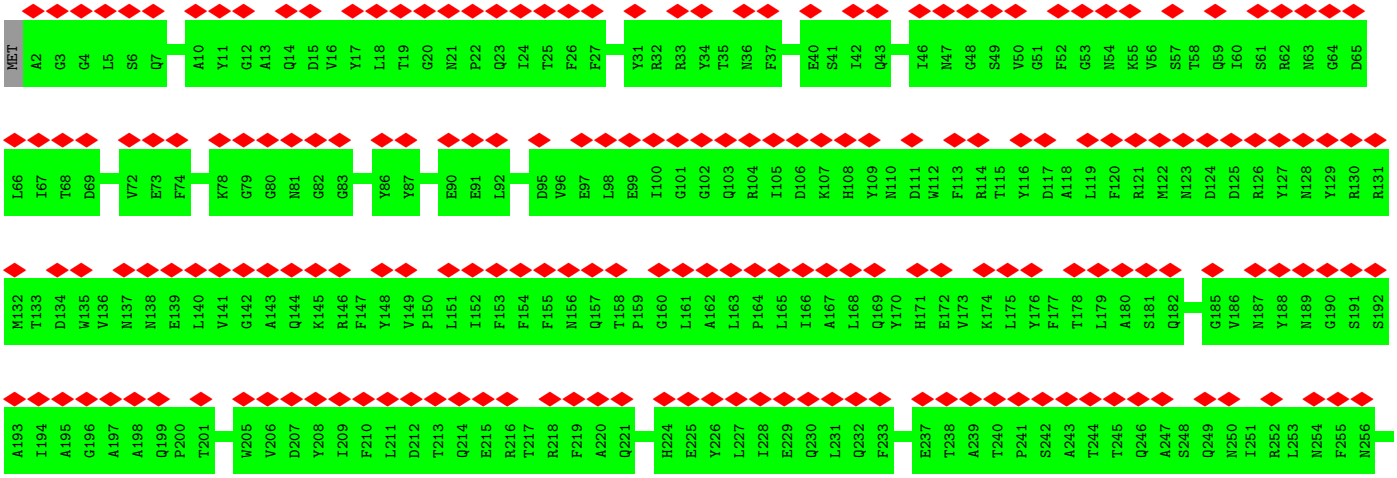
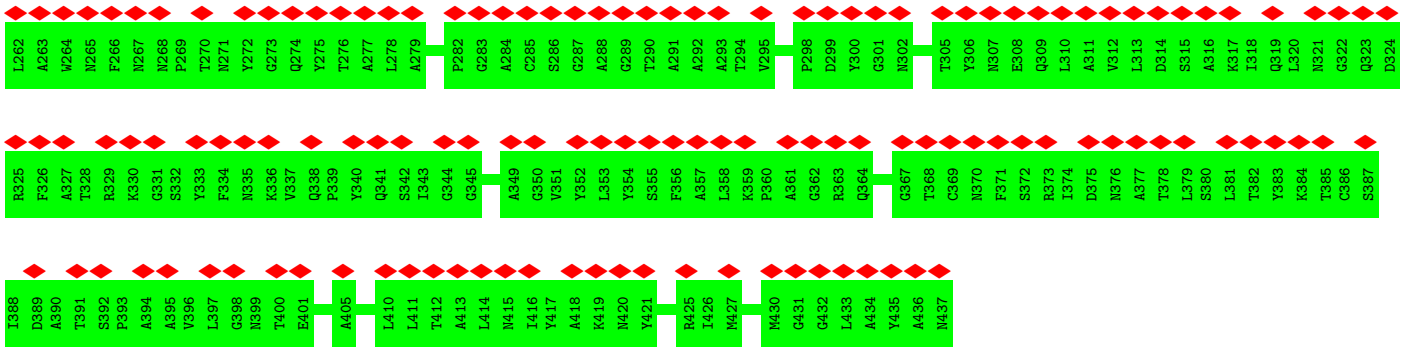
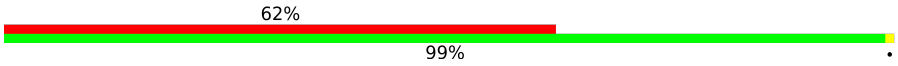
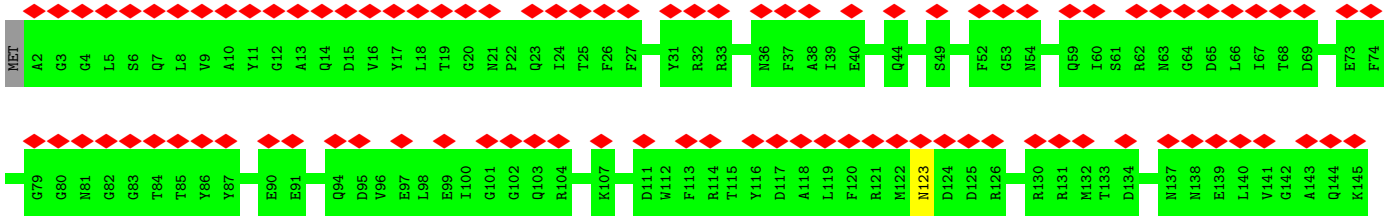




• Molecule 1: Major capsid protein (MCP)

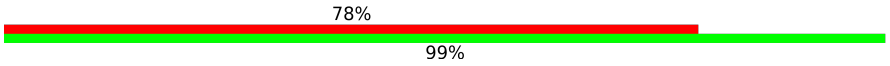
Chain ak:

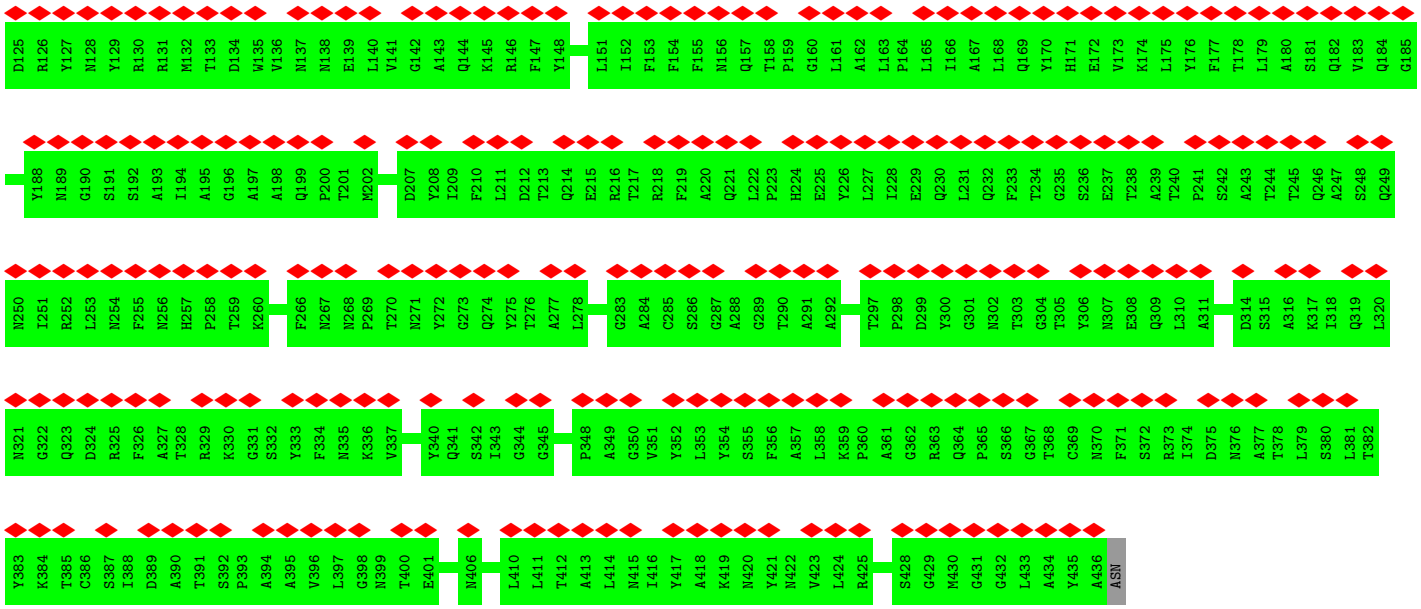




• Molecule 1: Major capsid protein (MCP)

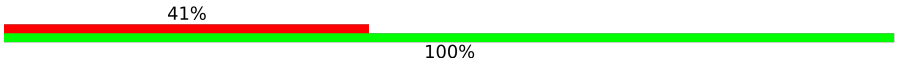
Chain al:

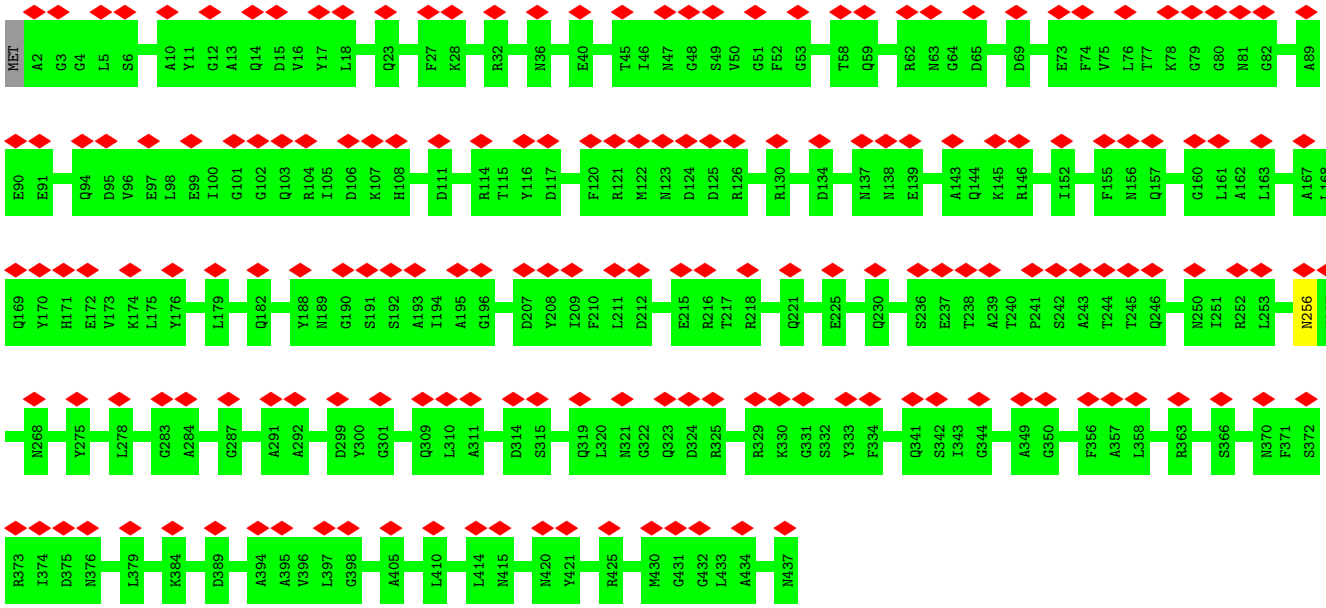




• Molecule 1: Major capsid protein (MCP)

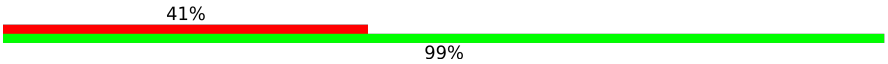
Chain am:

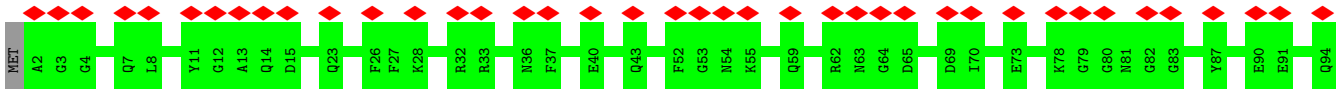


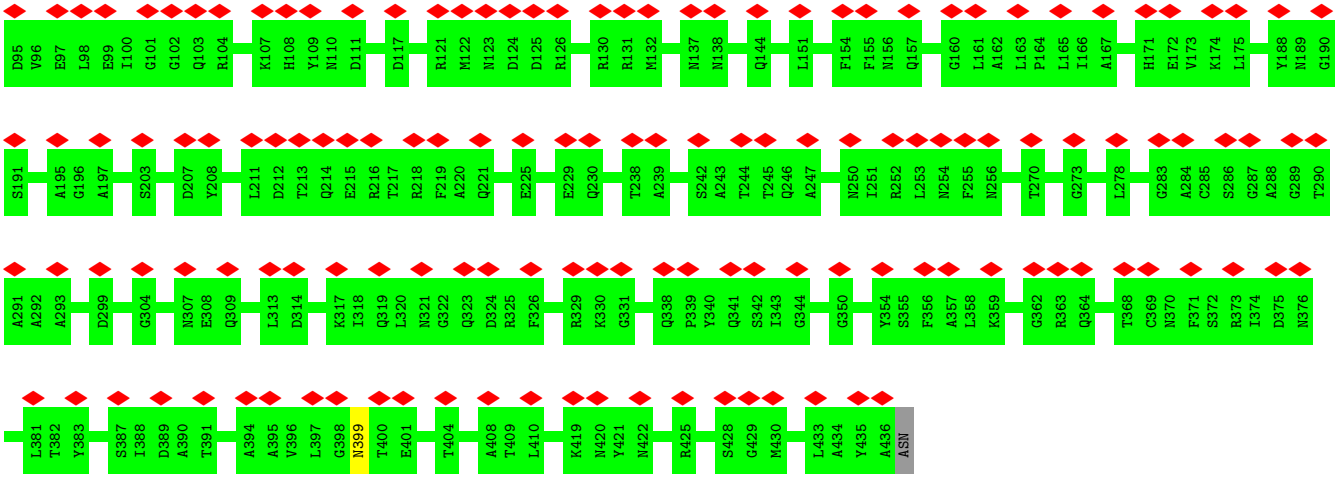


• Molecule 1: Major capsid protein (MCP)

Chain an:

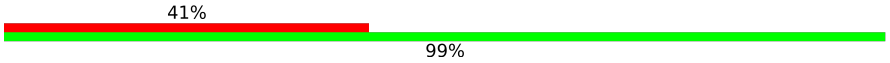


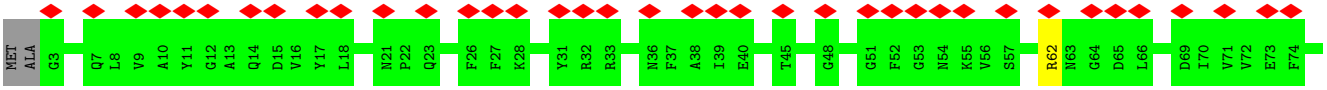


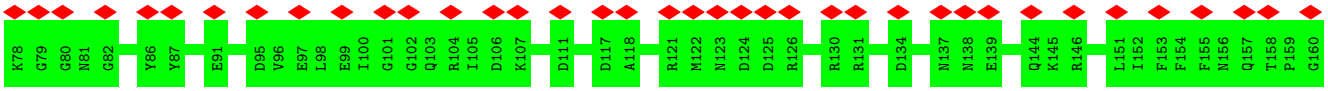


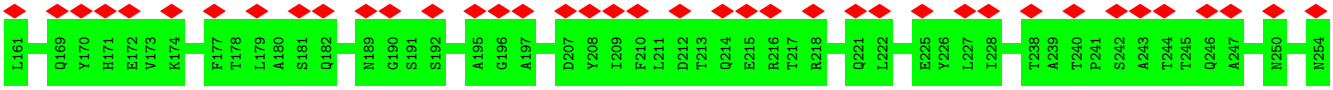
• Molecule 1: Major capsid protein (MCP)

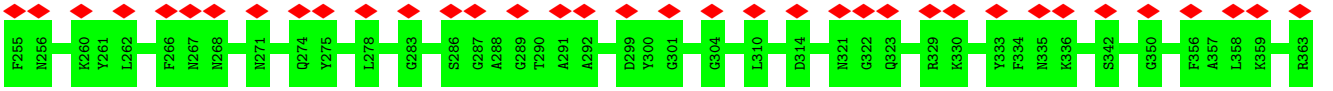
Chain ao:

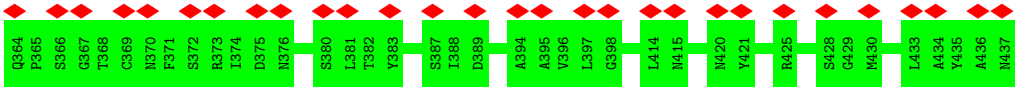






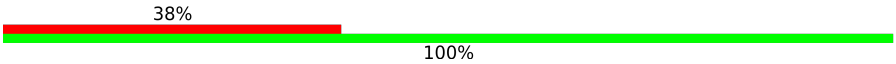


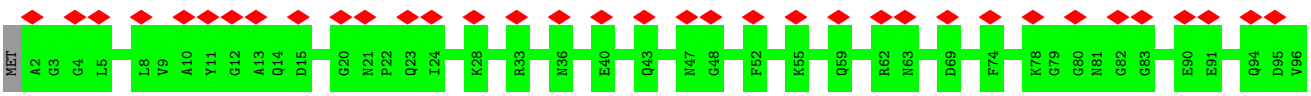


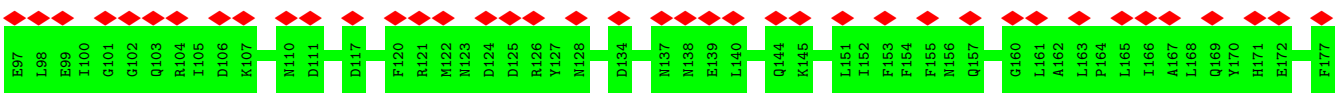


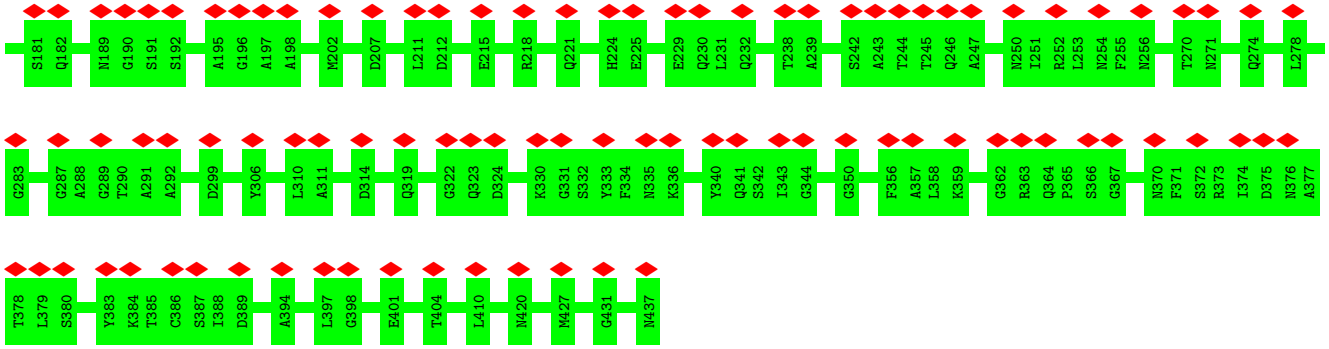
• Molecule 1: Major capsid protein (MCP)

Chain ap:



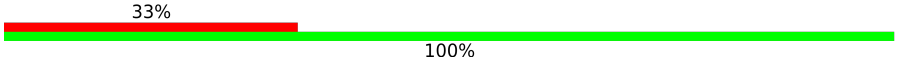


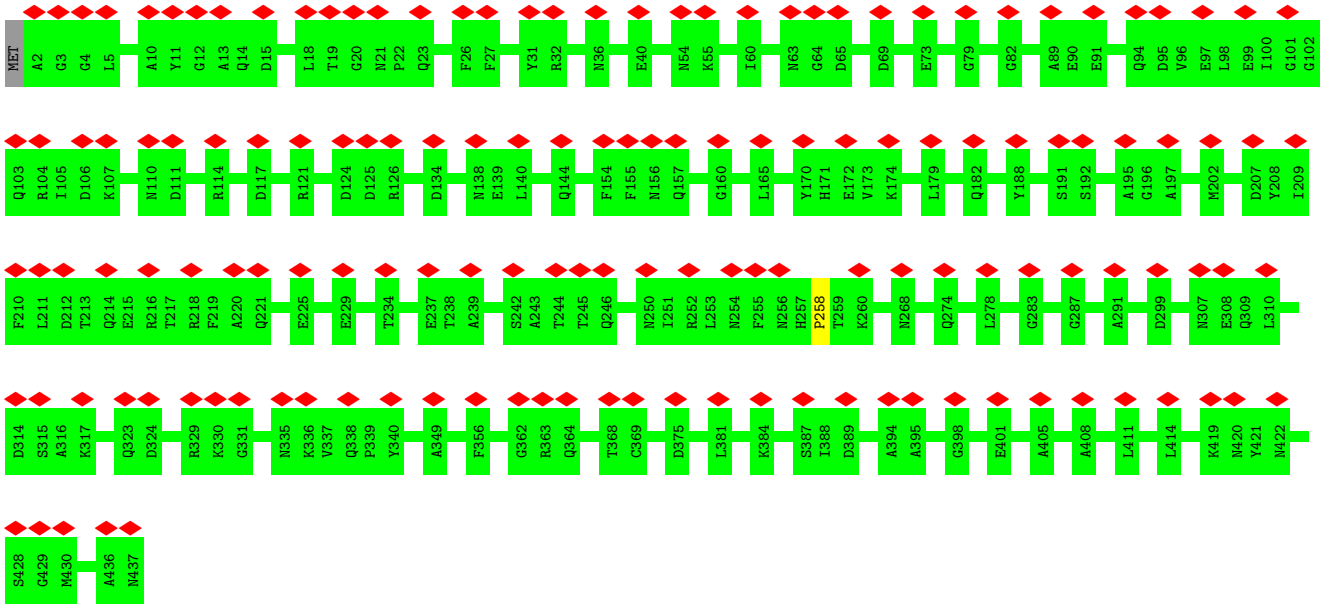




• Molecule 1: Major capsid protein (MCP)

Chain aq:





• Molecule 1: Major capsid protein (MCP)

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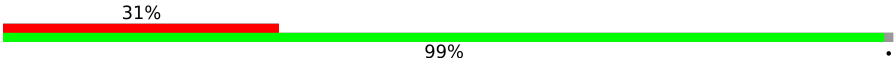
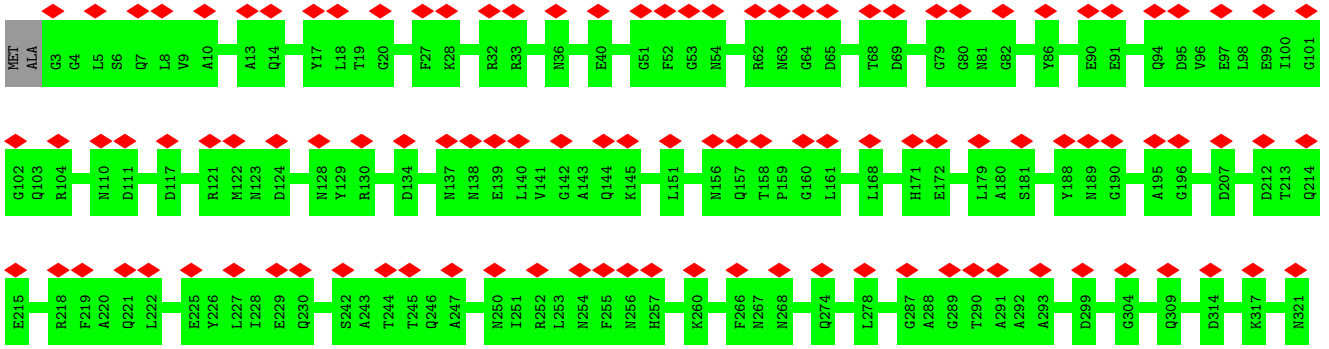
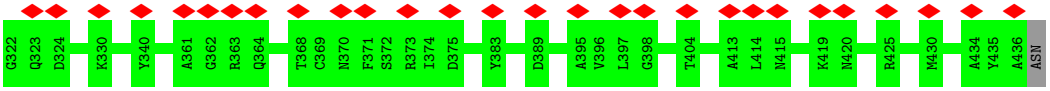
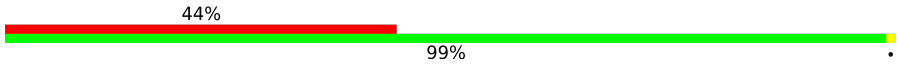






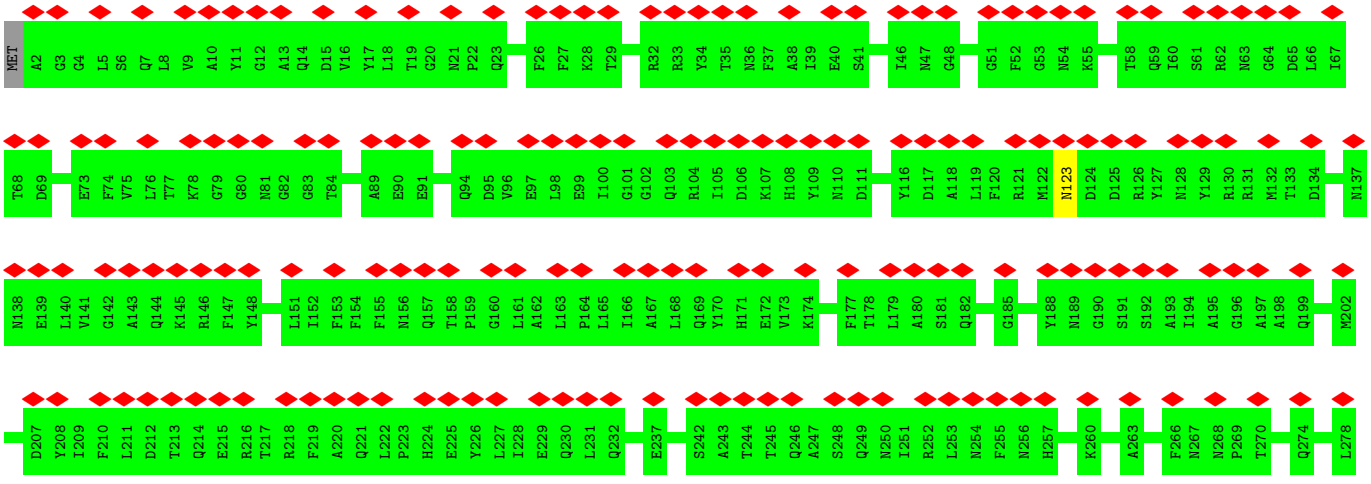
• Molecule 1: Major capsid protein (MCP)

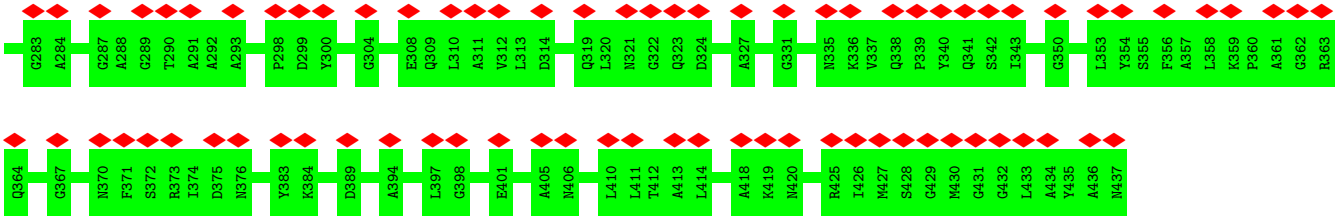
Chain as:



• Molecule 1: Major capsid protein (MCP)

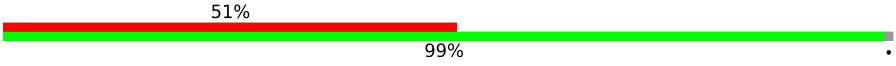
Chain at:

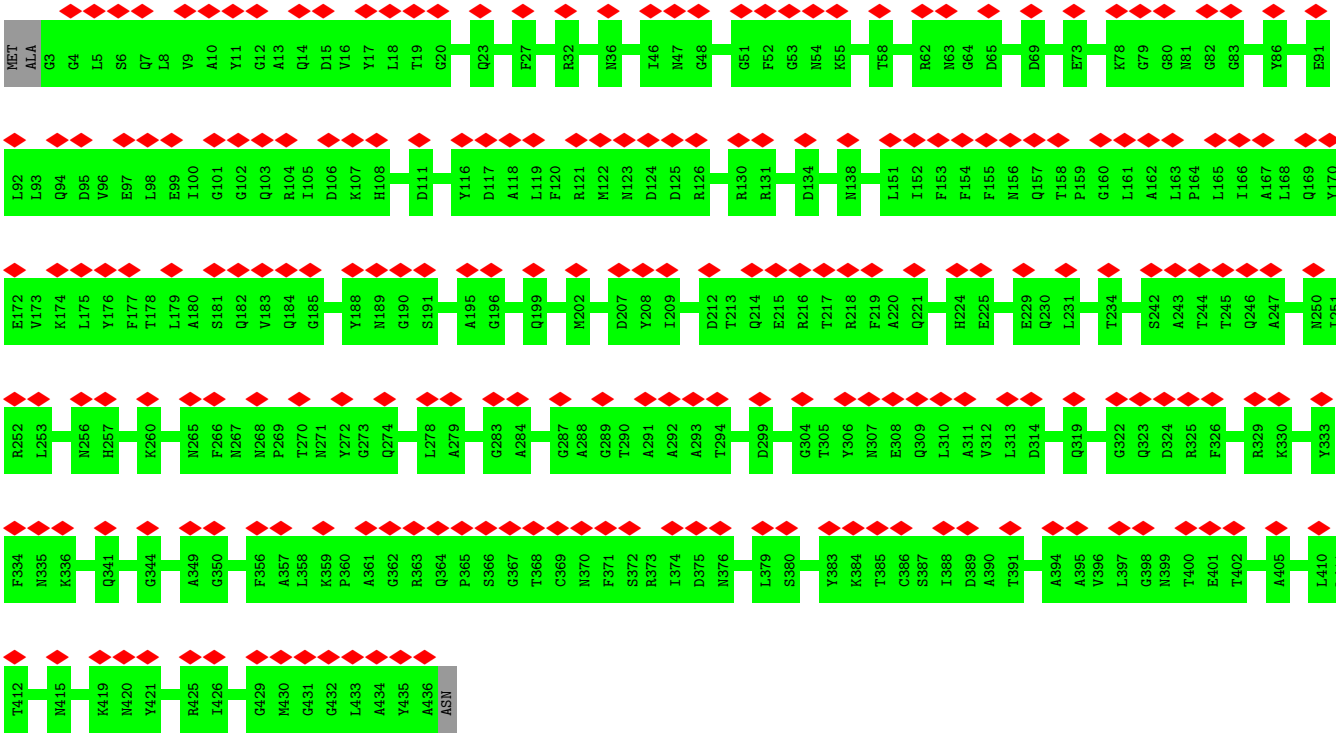




• Molecule 1: Major capsid protein (MCP)

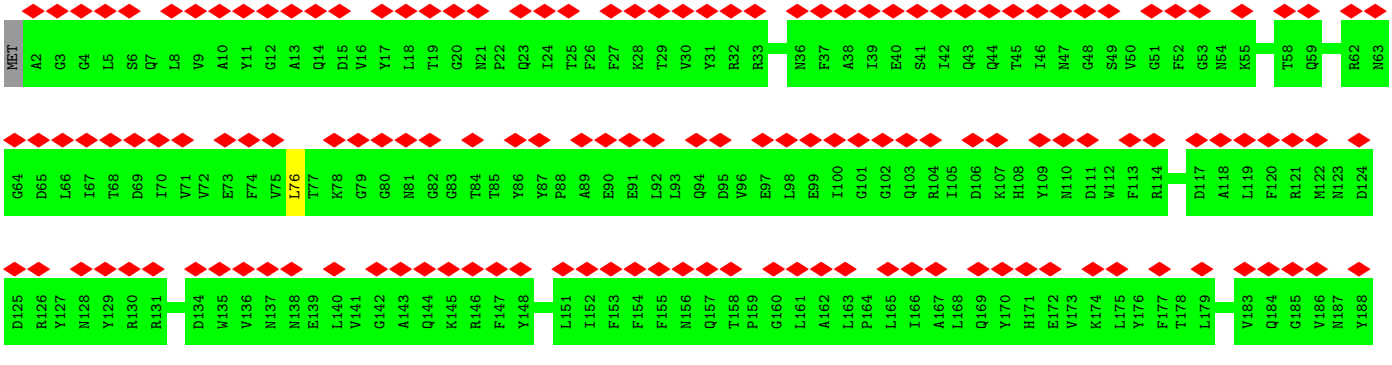
Chain au:

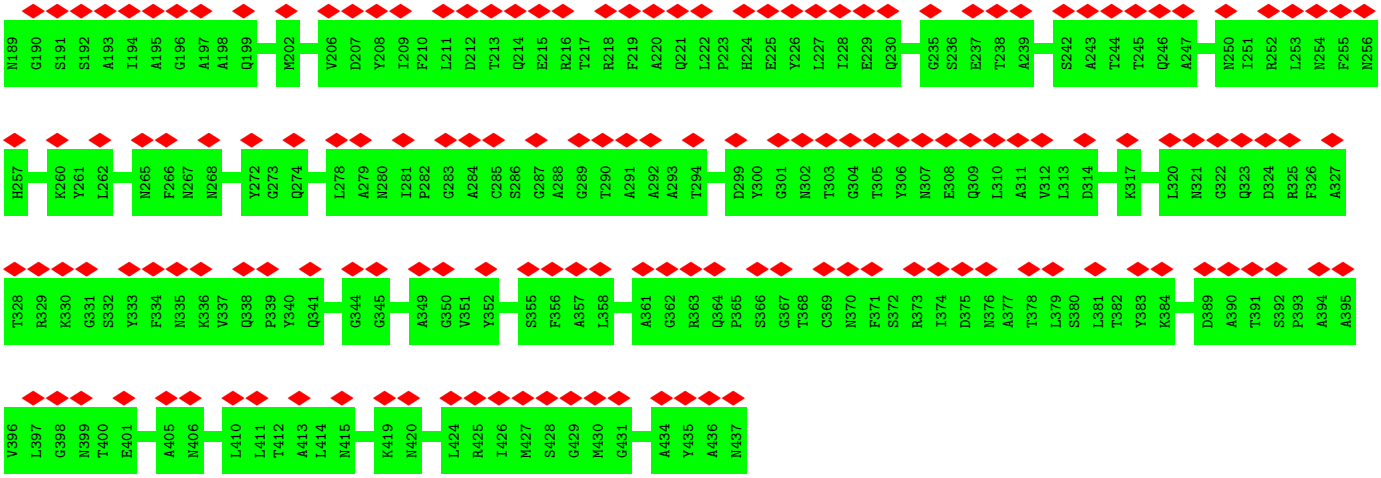




• Molecule 1: Major capsid protein (MCP)

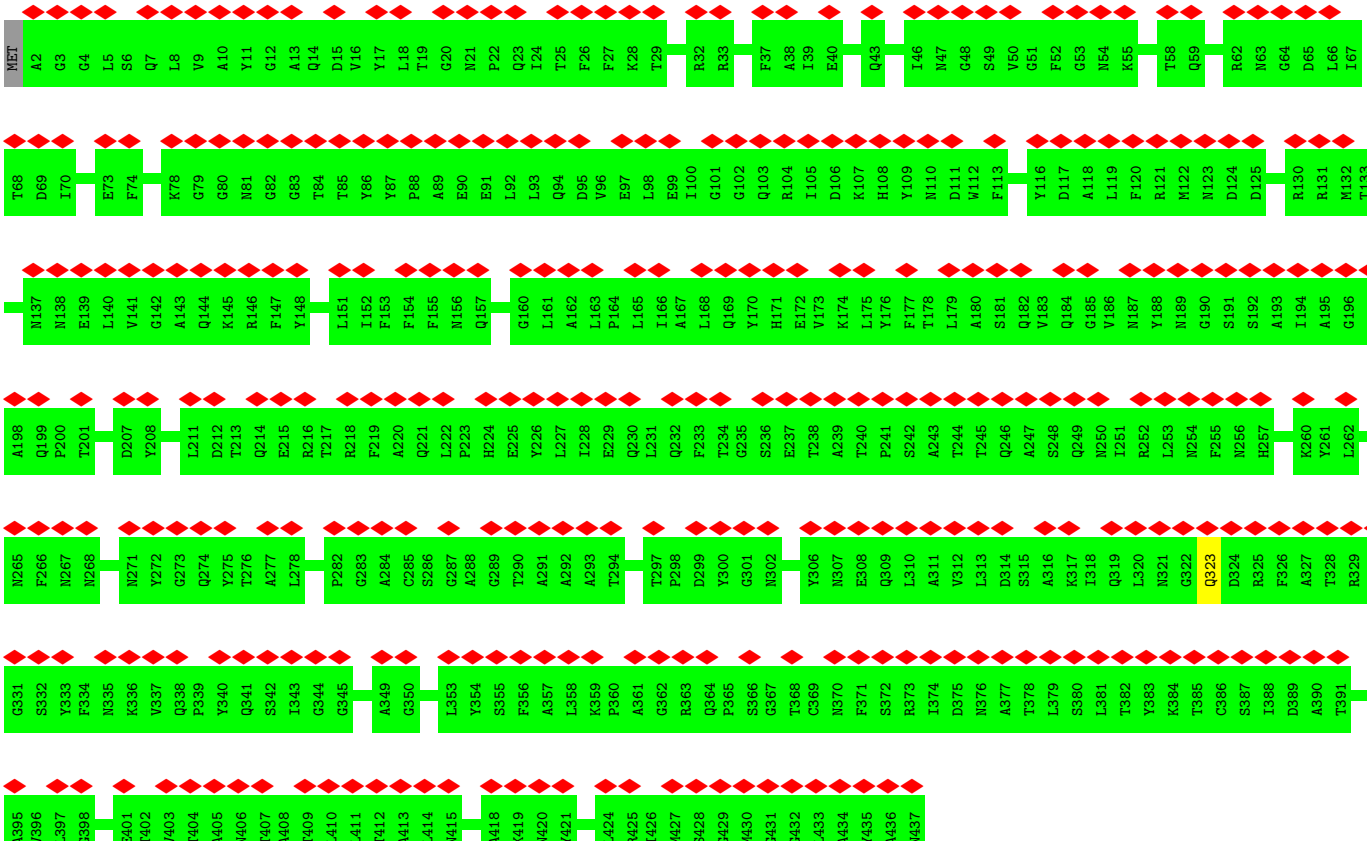
Chain av:





• Molecule 1: Major capsid protein (MCP)

Chain aw:



• Molecule 1: Major capsid protein (MCP)

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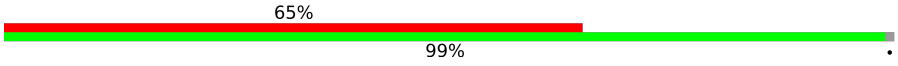
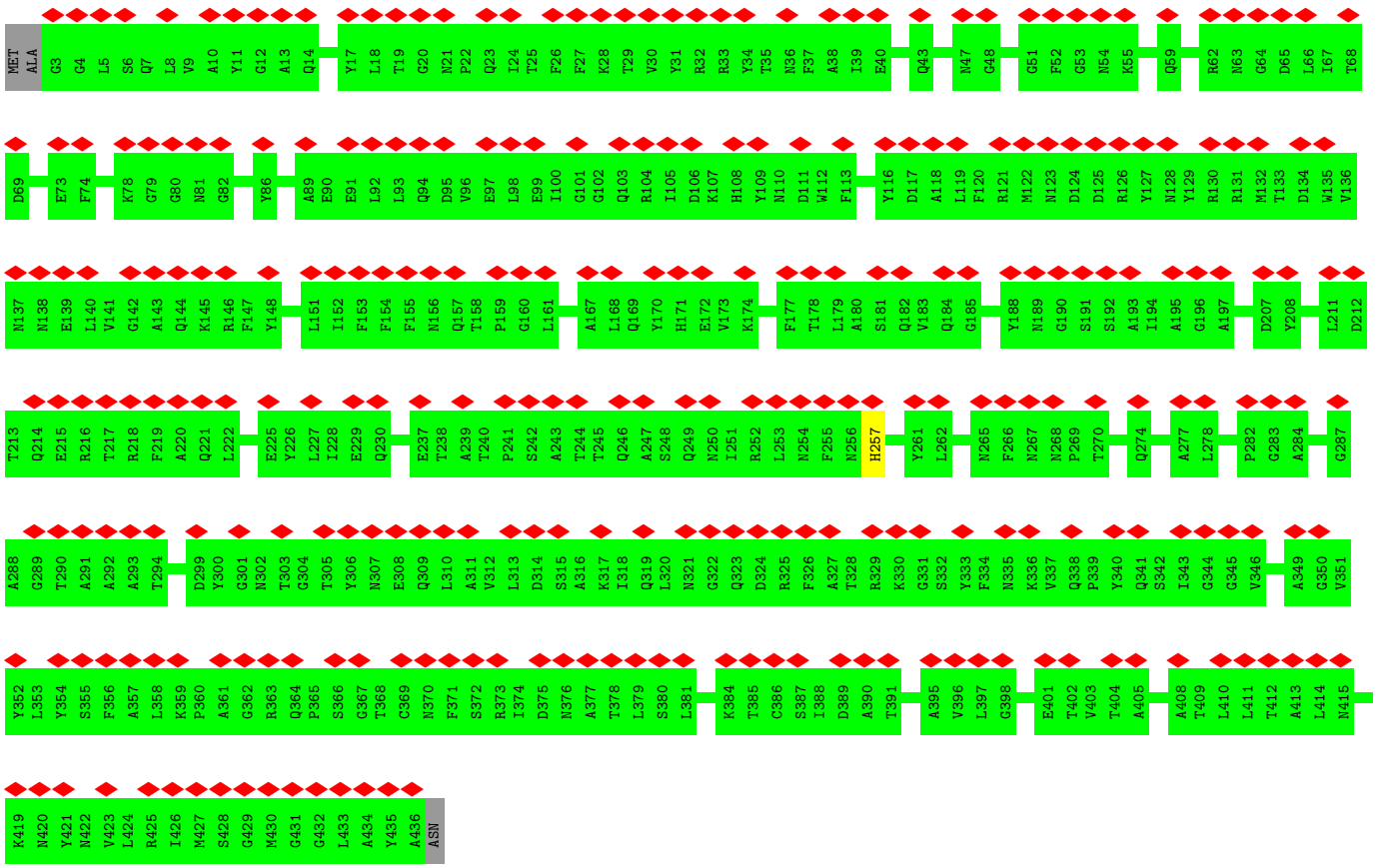
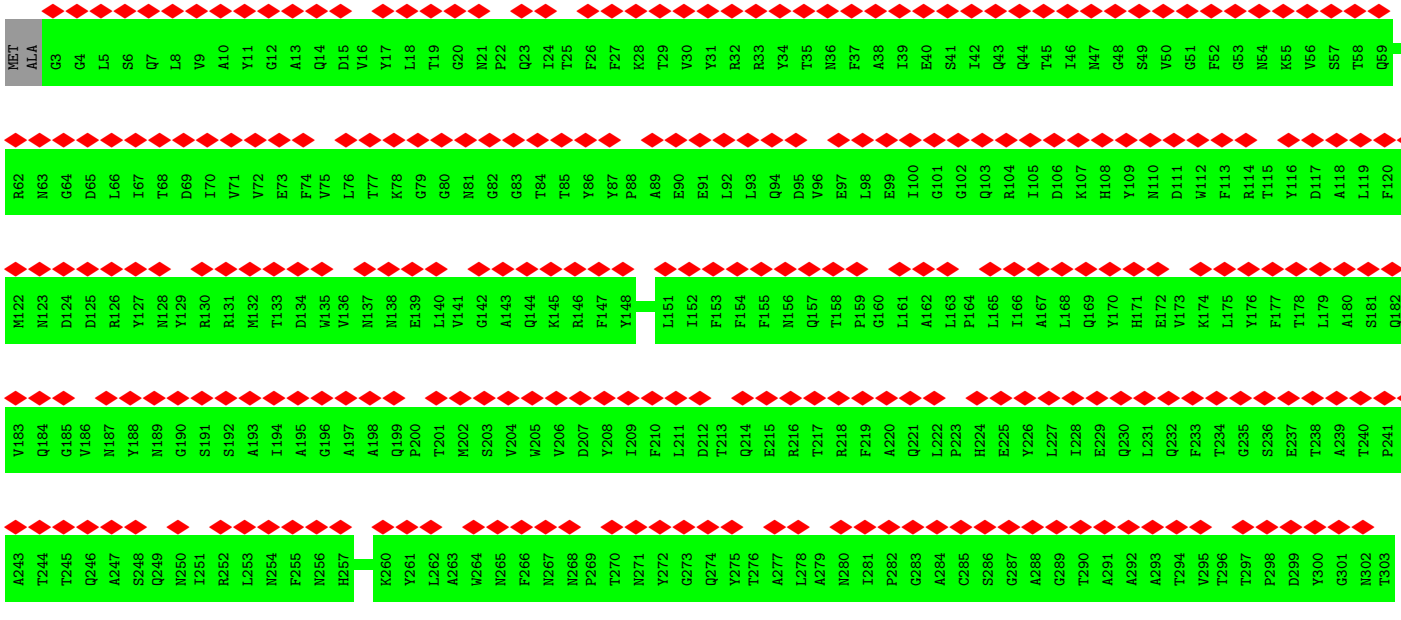
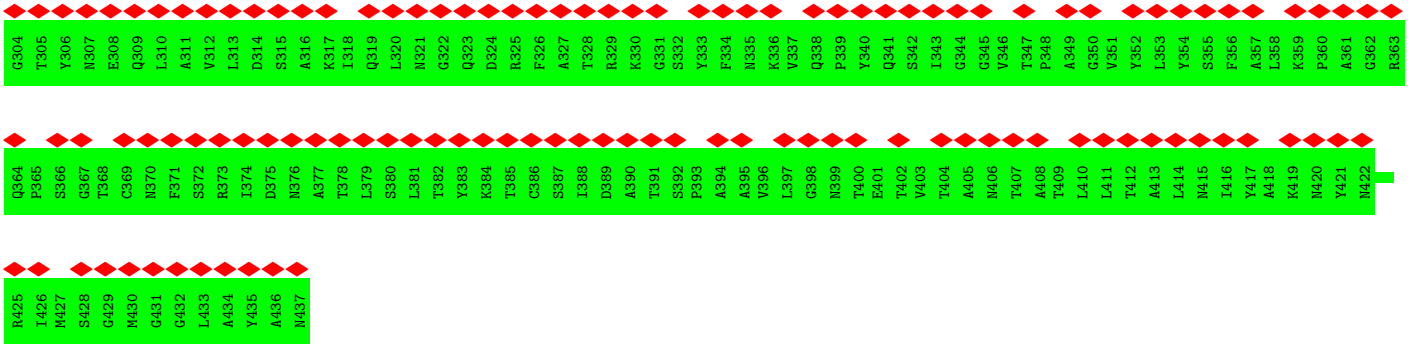




• Molecule 1: Major capsid protein (MCP)

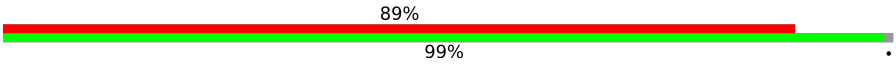
Chain ay:

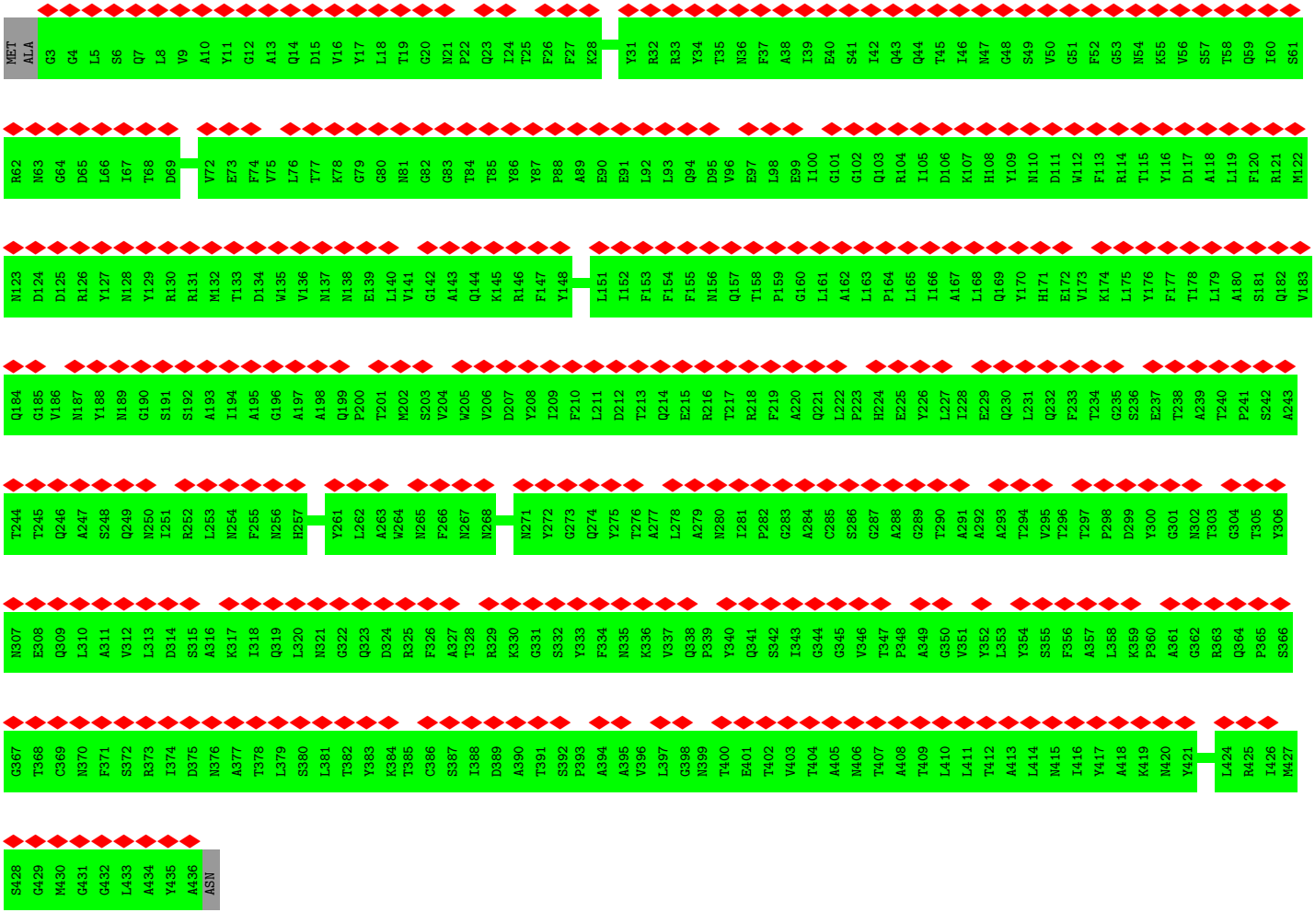




• Molecule 1: Major capsid protein (MCP)

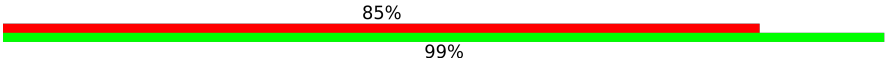
Chain az:

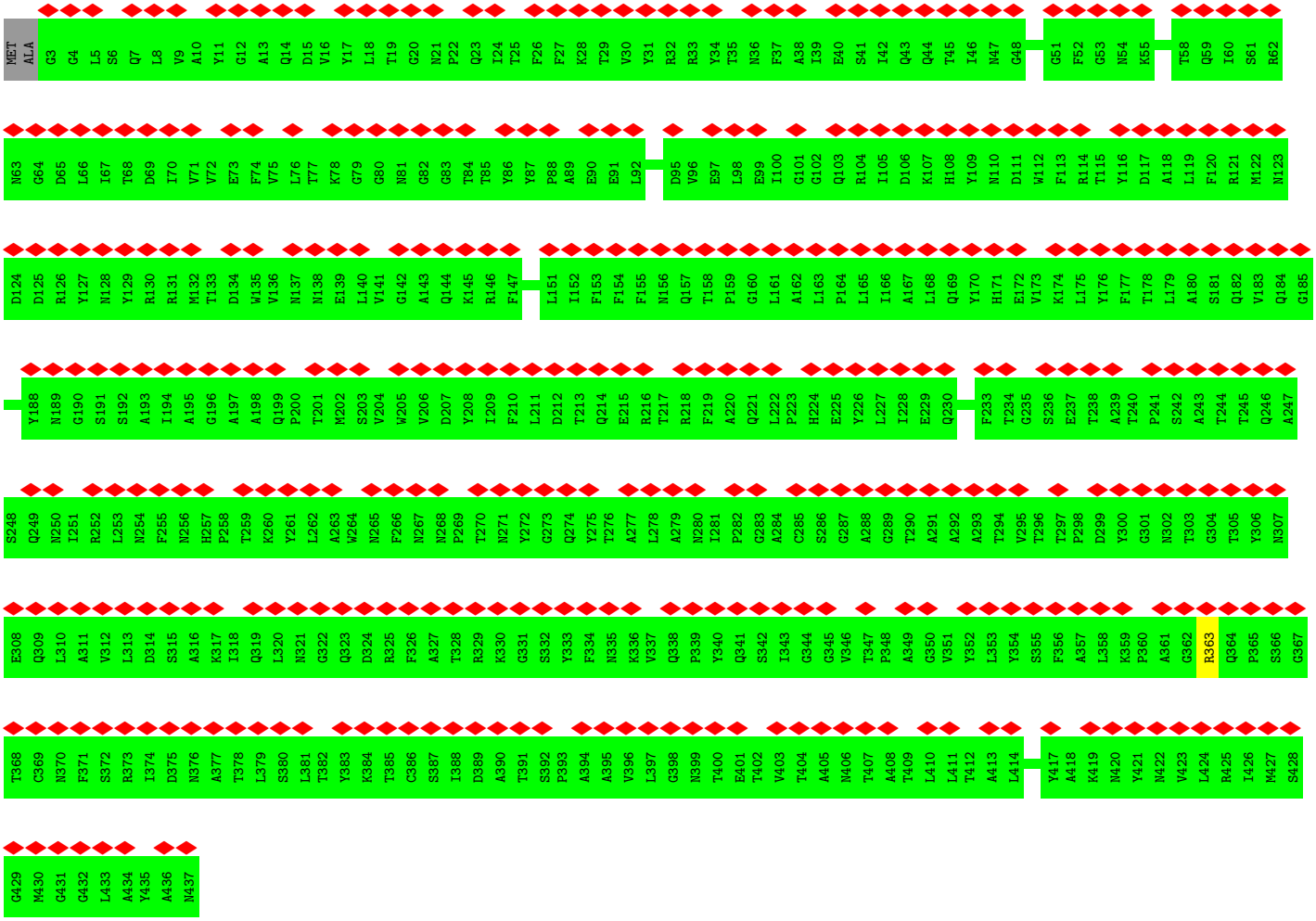




• Molecule 1: Major capsid protein (MCP)

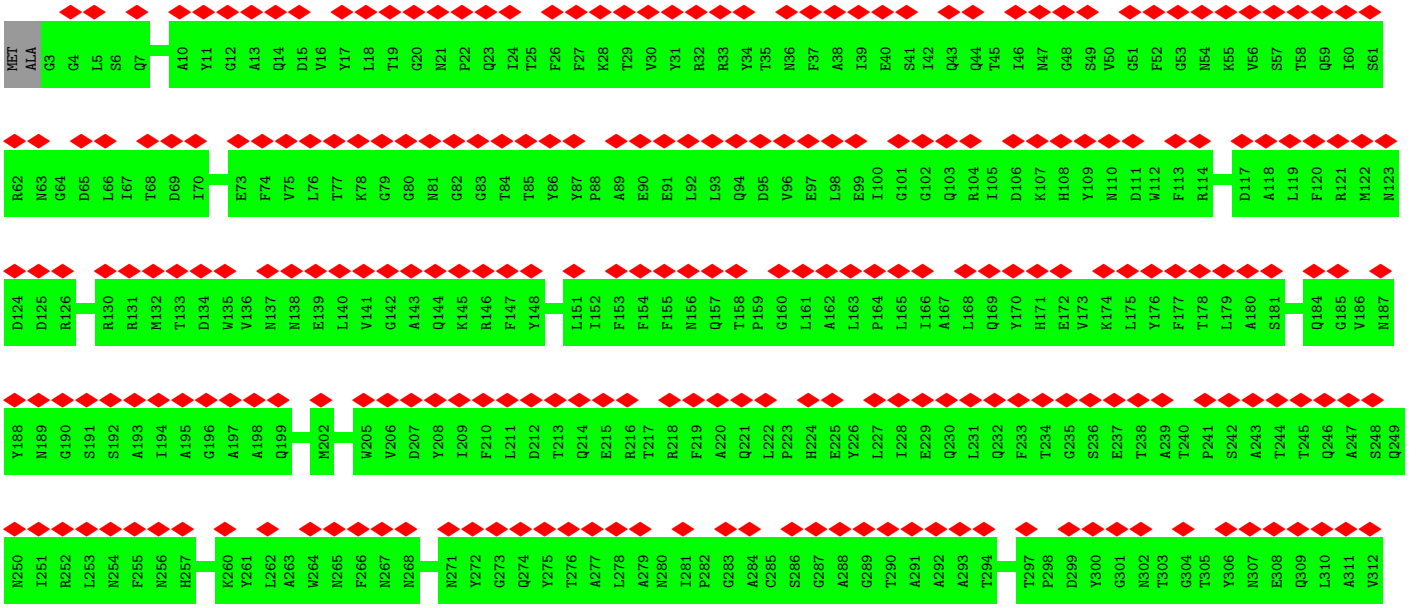
Chain aA:

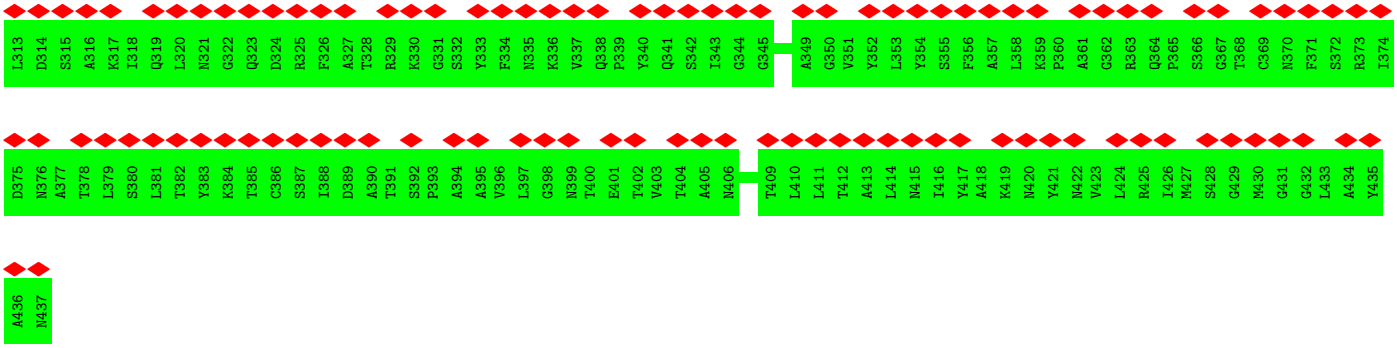




• Molecule 1: Major capsid protein (MCP)

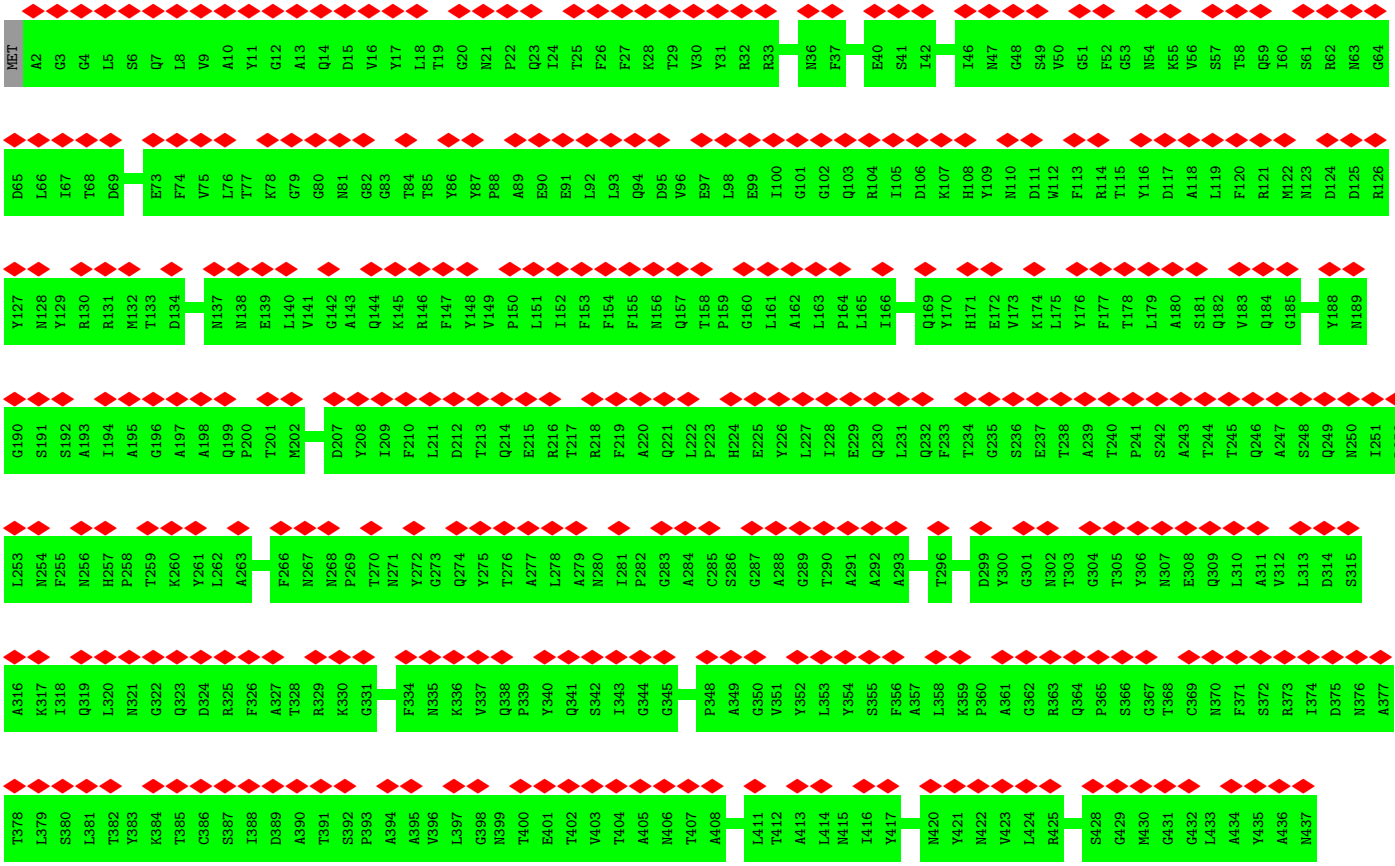
Chain aB:





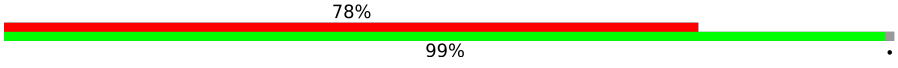
• Molecule 1: Major capsid protein (MCP)

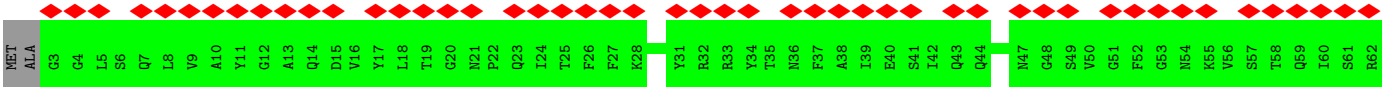
Chain aC:

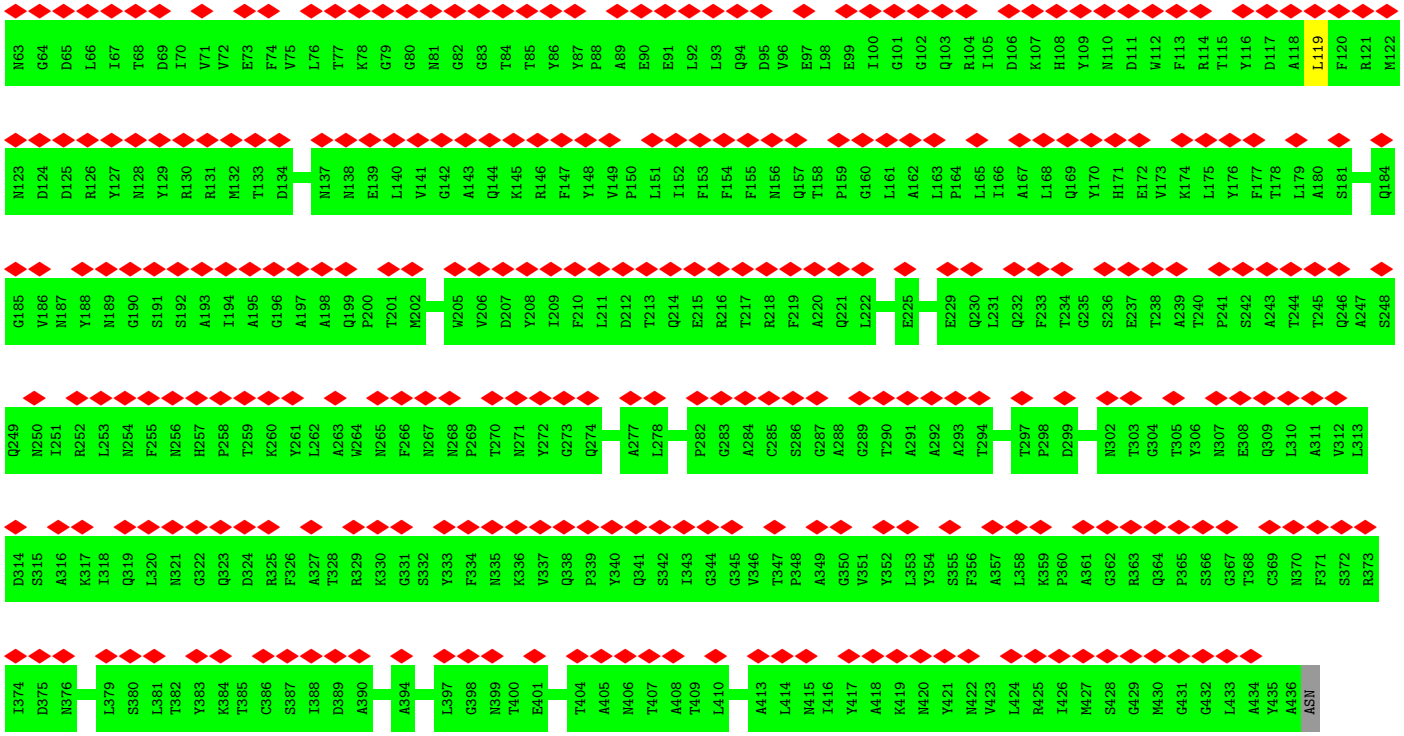


• Molecule 1: Major capsid protein (MCP)

Chain aD:

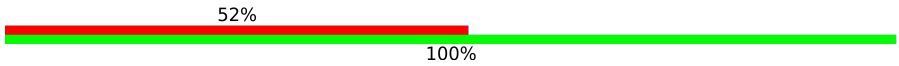






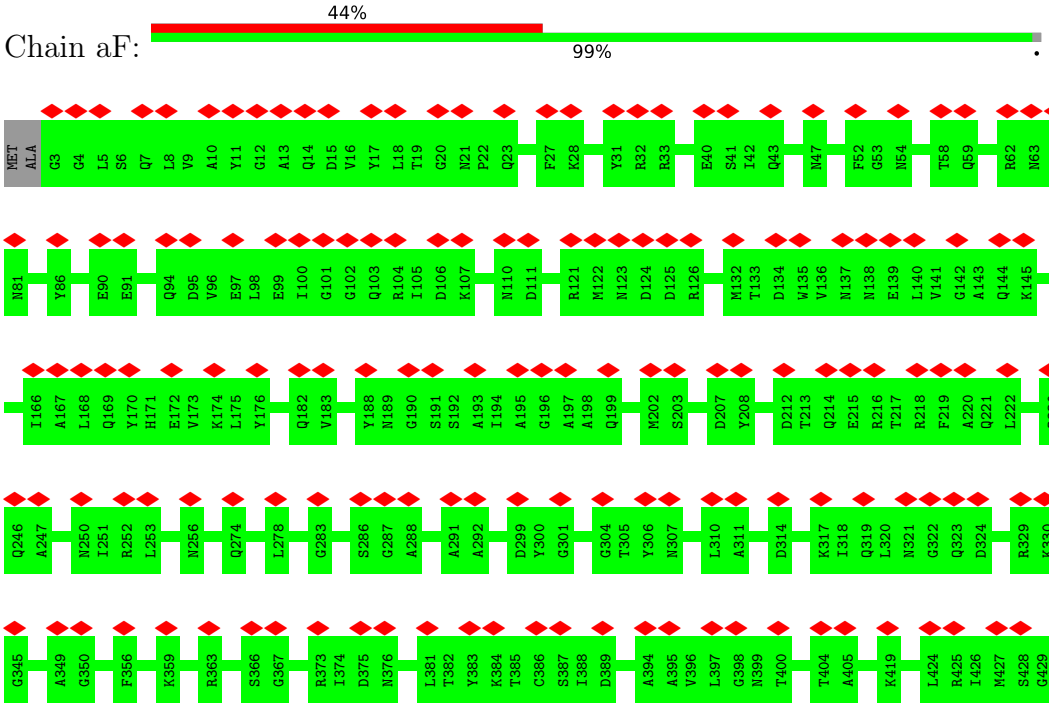
• Molecule 1: Major capsid protein (MCP)

Chain aE:



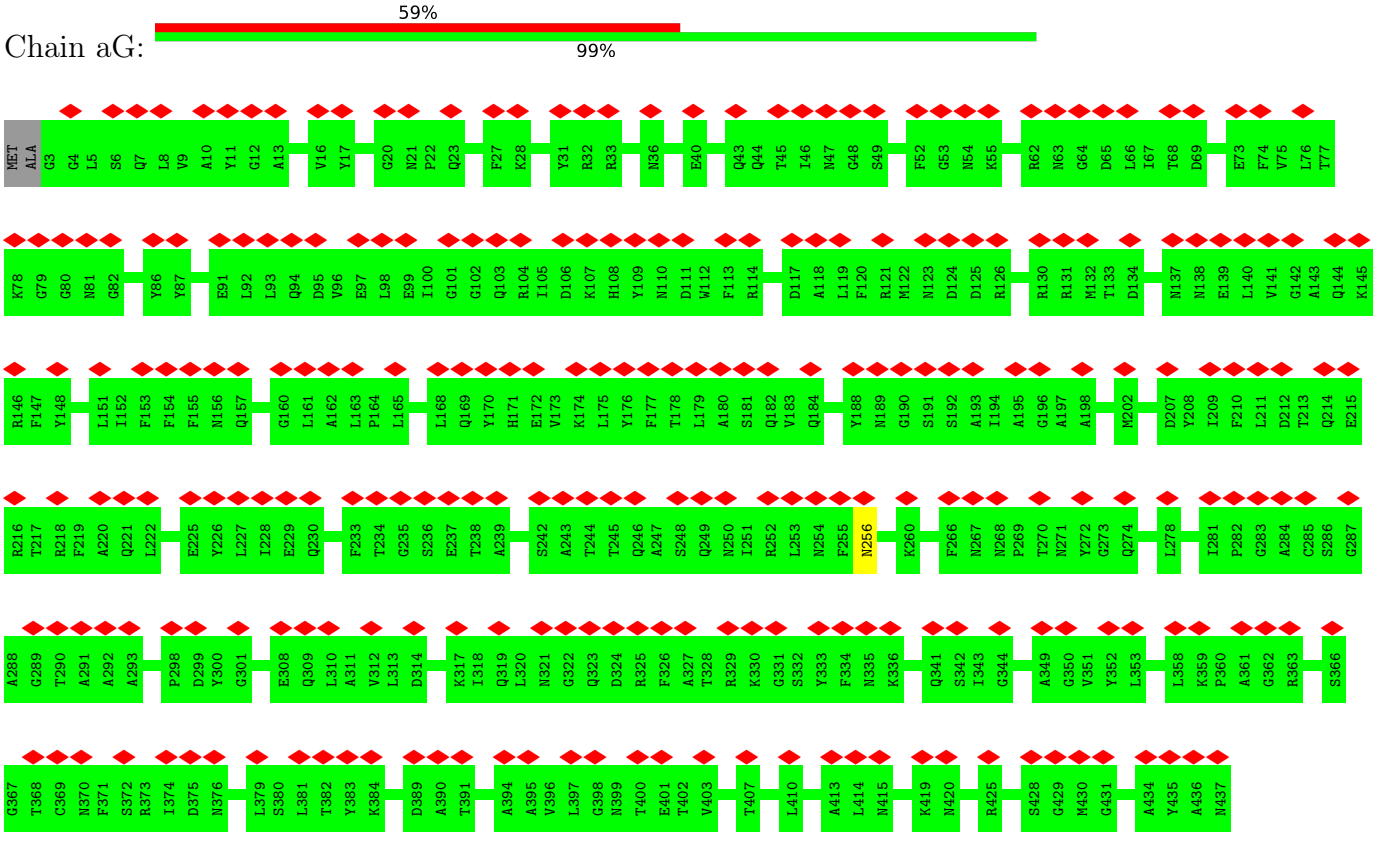
• Molecule 1: Major capsid protein (MCP)

Chain aF:



• Molecule 1: Major capsid protein (MCP)

Chain aG:

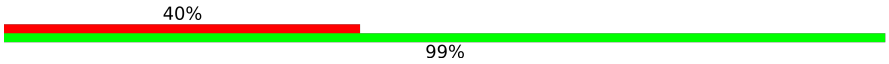


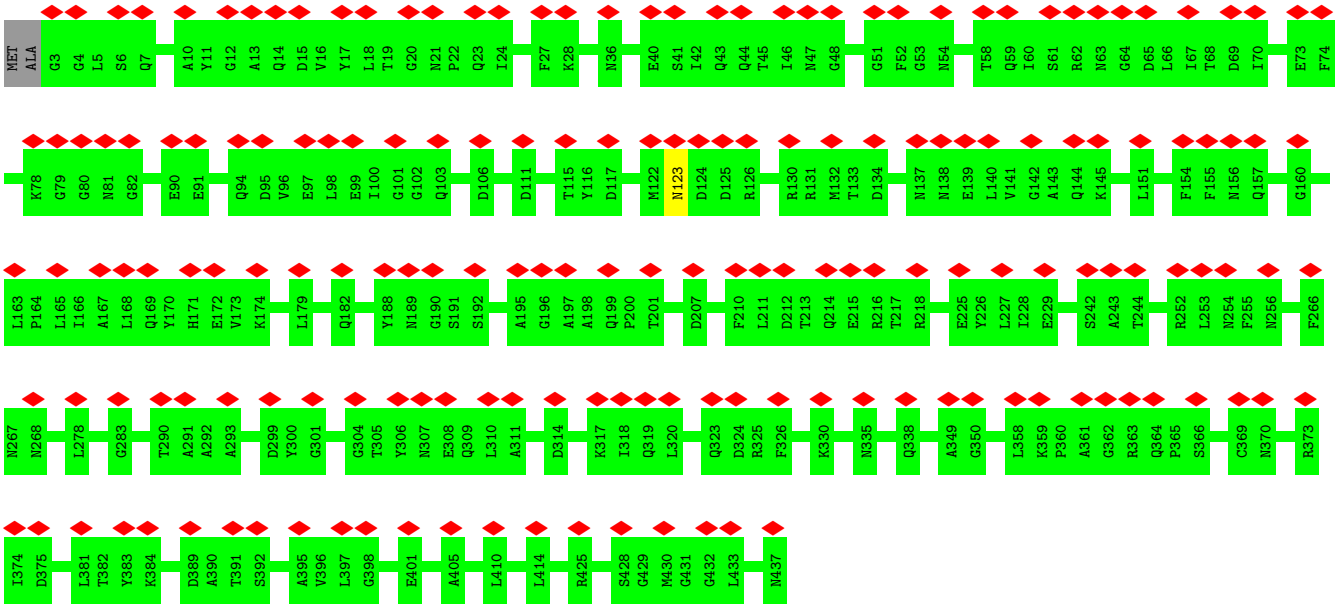
• Molecule 1: Major capsid protein (MCP)

Chain aH:

• Molecule 1: Major capsid protein (MCP)

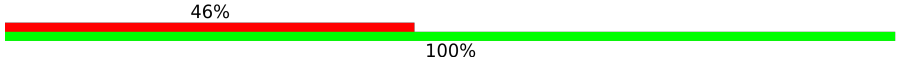
Chain aI:

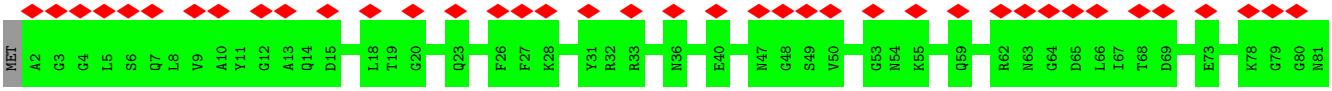


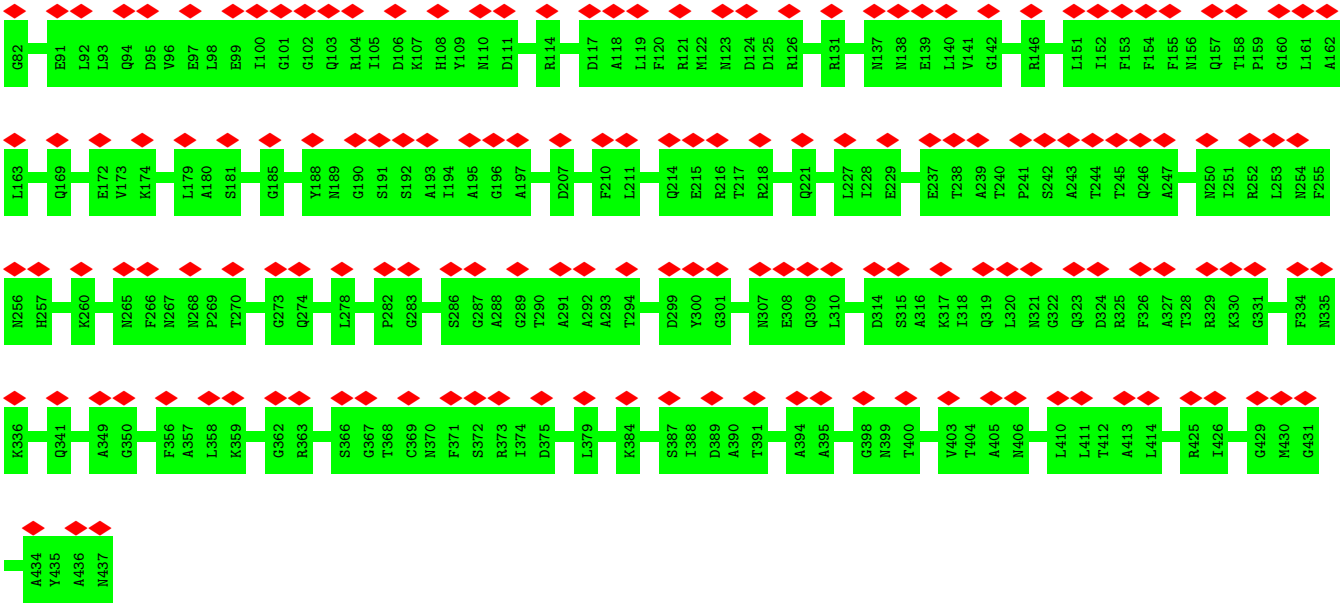


• Molecule 1: Major capsid protein (MCP)

Chain aJ:

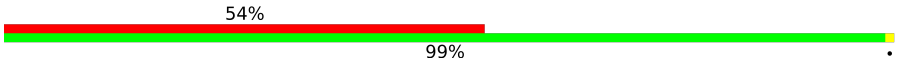


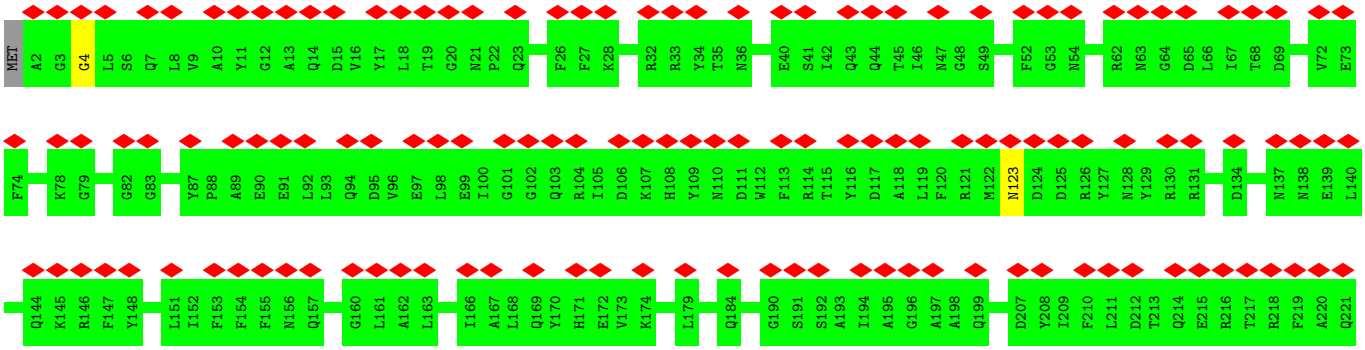




• Molecule 1: Major capsid protein (MCP)

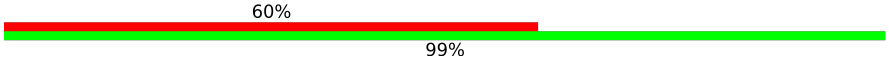
Chain aK:

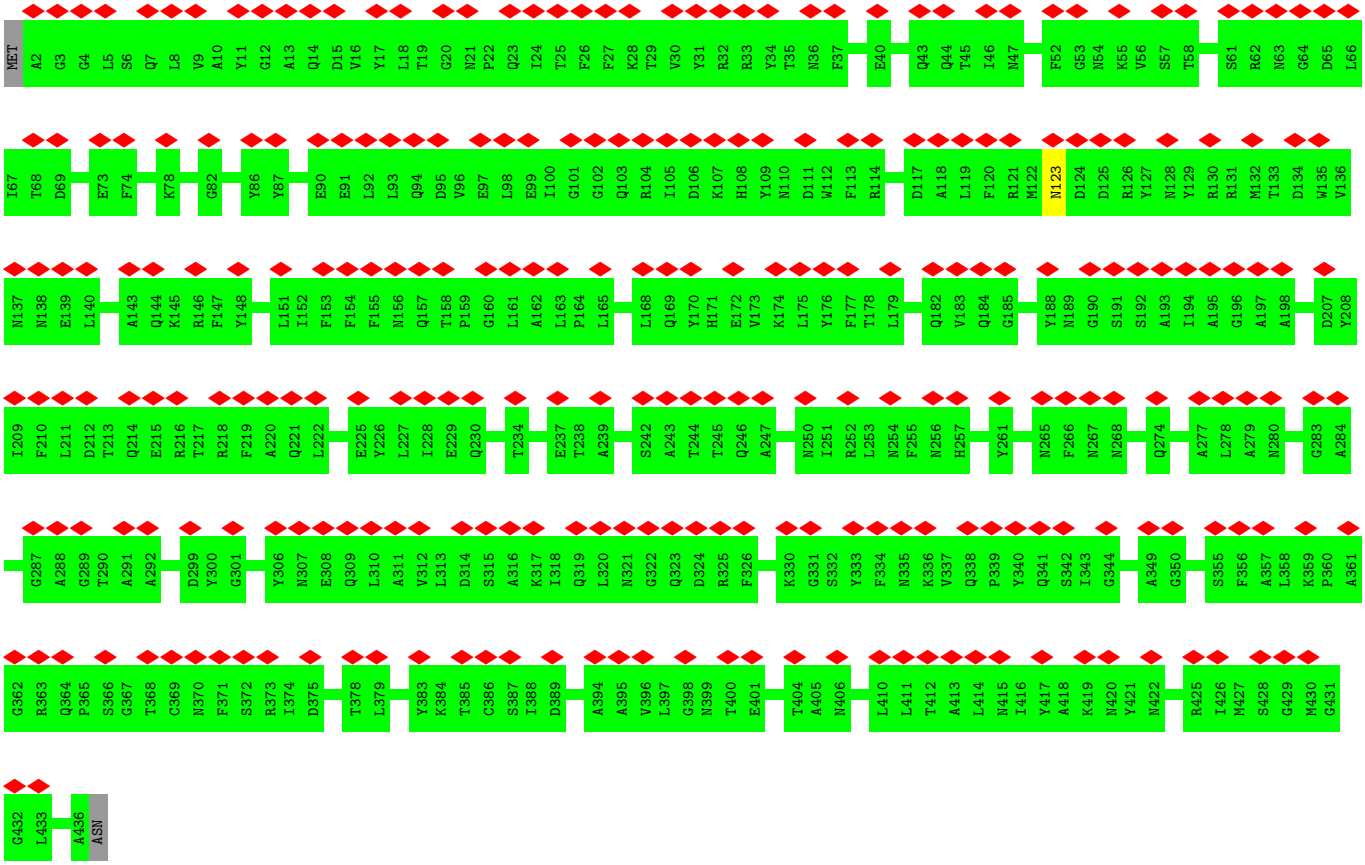




• Molecule 1: Major capsid protein (MCP)

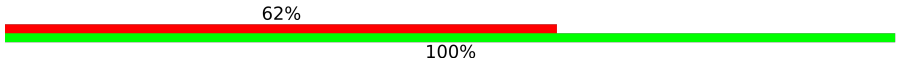
Chain aL:

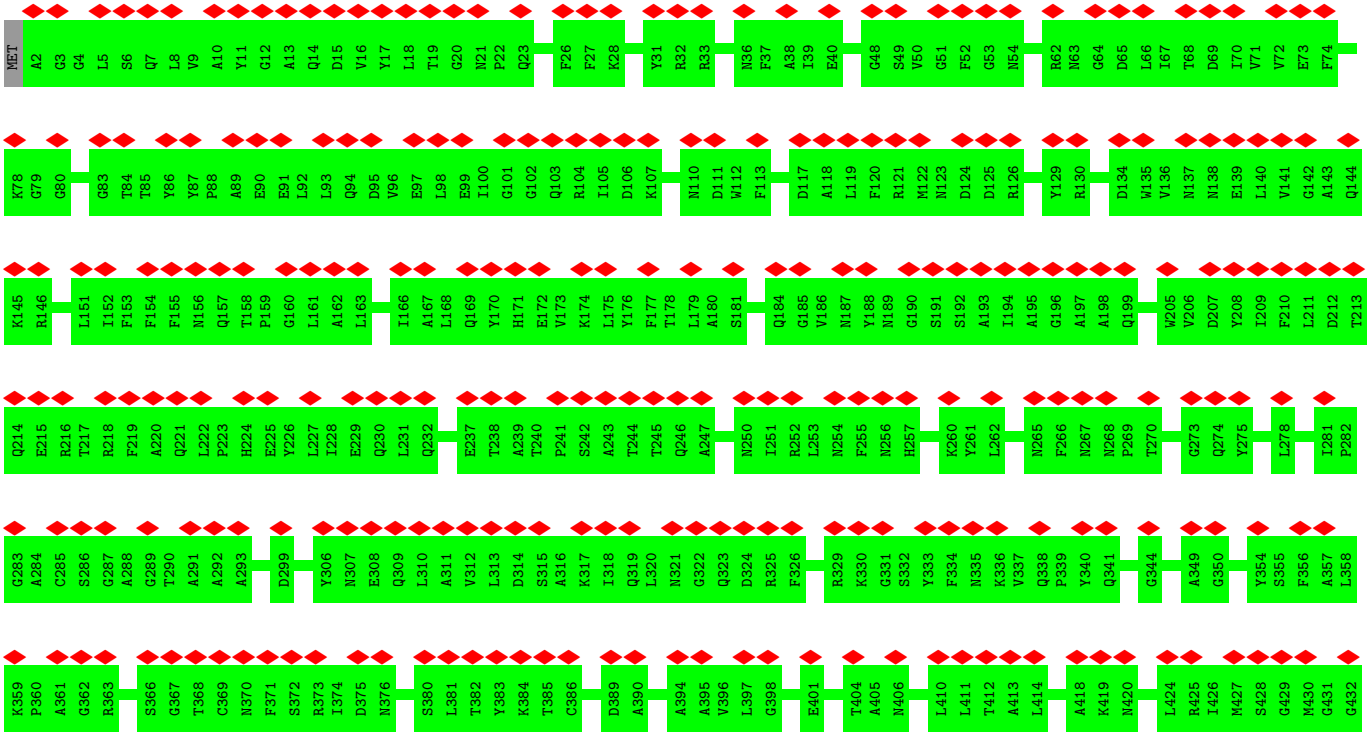


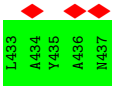


• Molecule 1: Major capsid protein (MCP)

Chain aM:

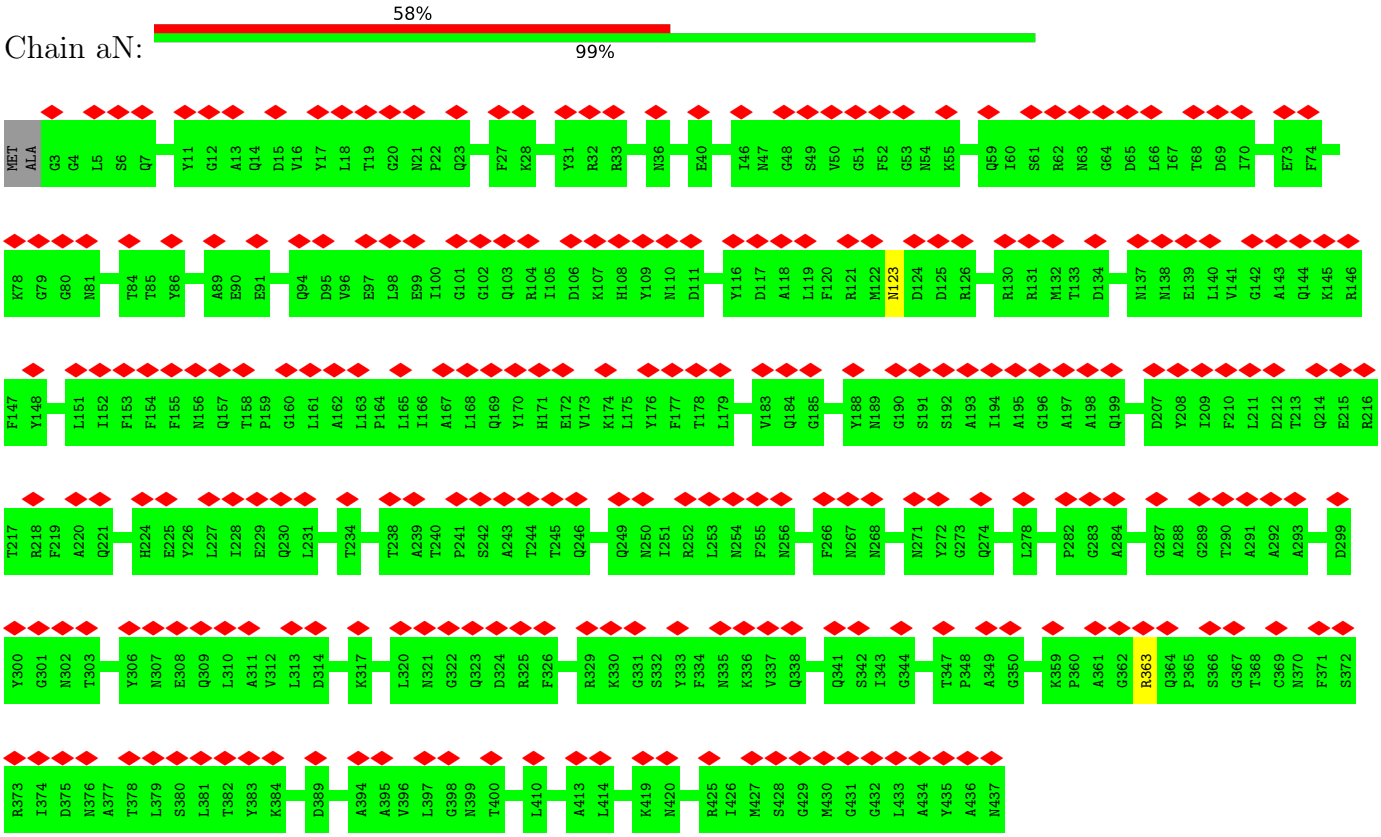






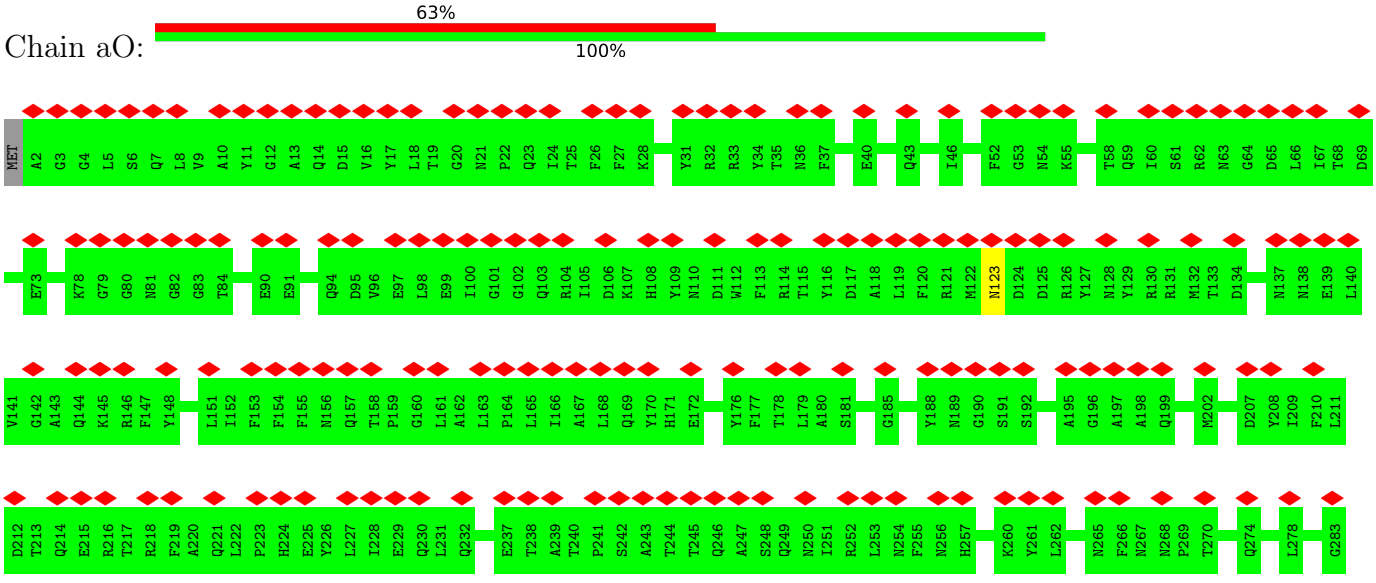
• Molecule 1: Major capsid protein (MCP)

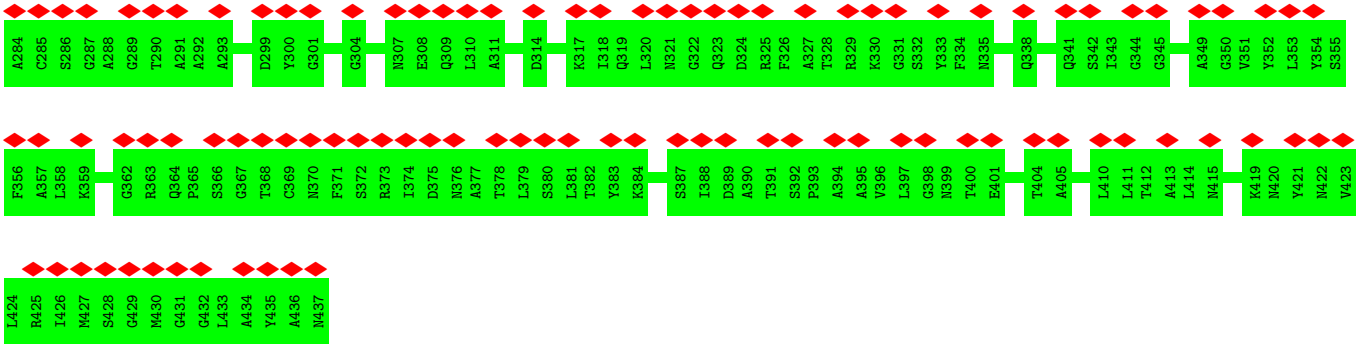
Chain aN:



• Molecule 1: Major capsid protein (MCP)

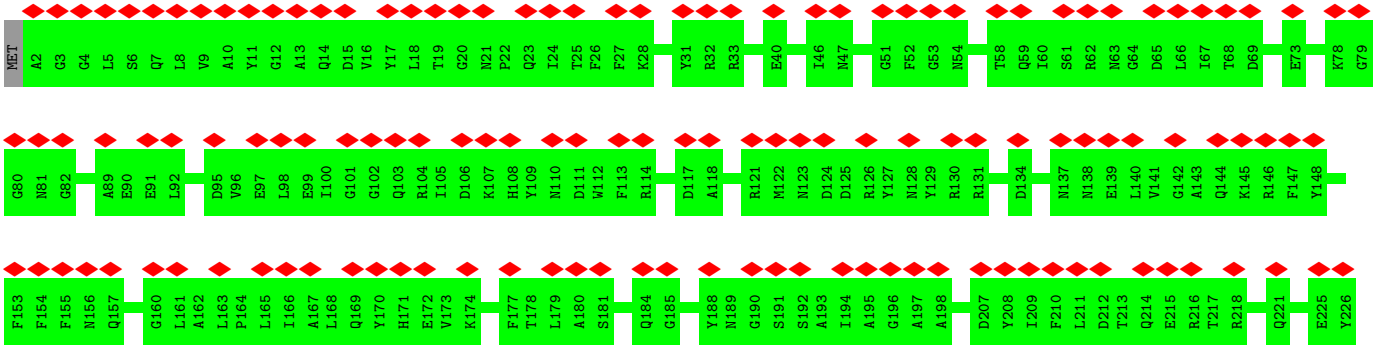
Chain aO:





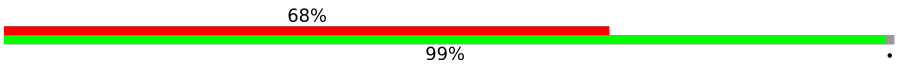
• Molecule 1: Major capsid protein (MCP)

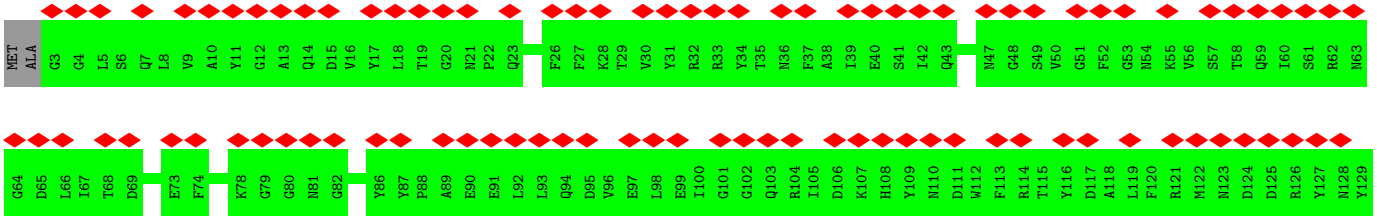
Chain aP:

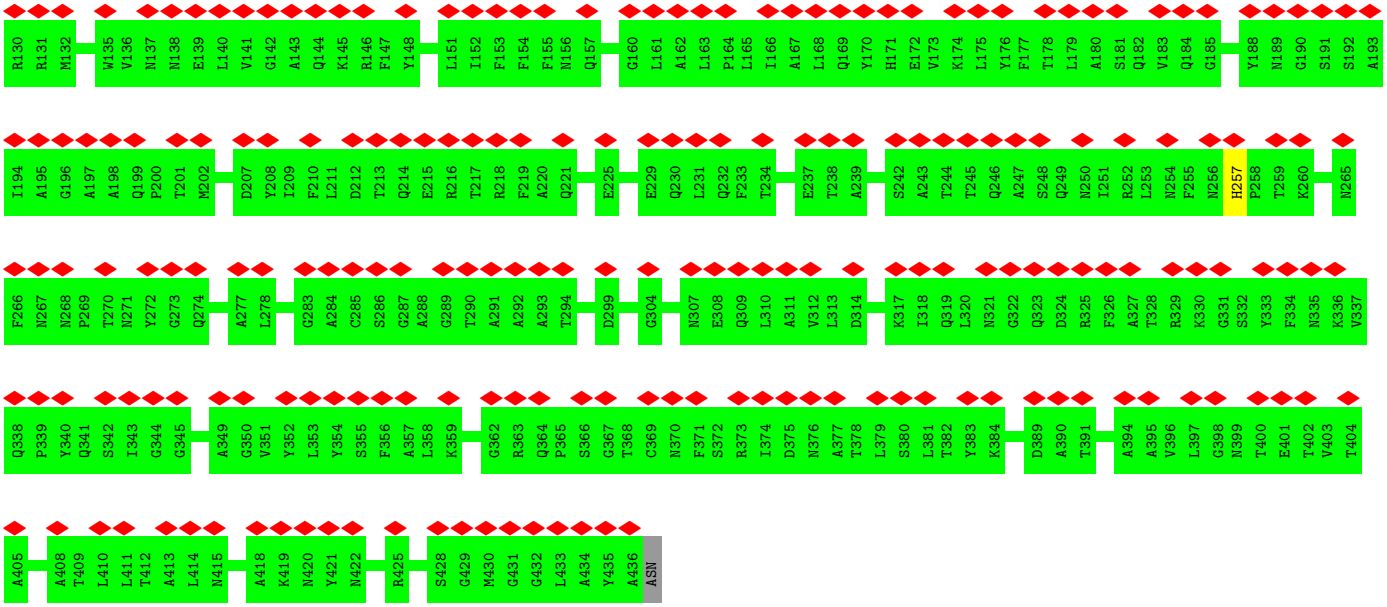


• Molecule 1: Major capsid protein (MCP)

Chain aQ:

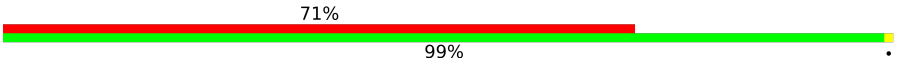


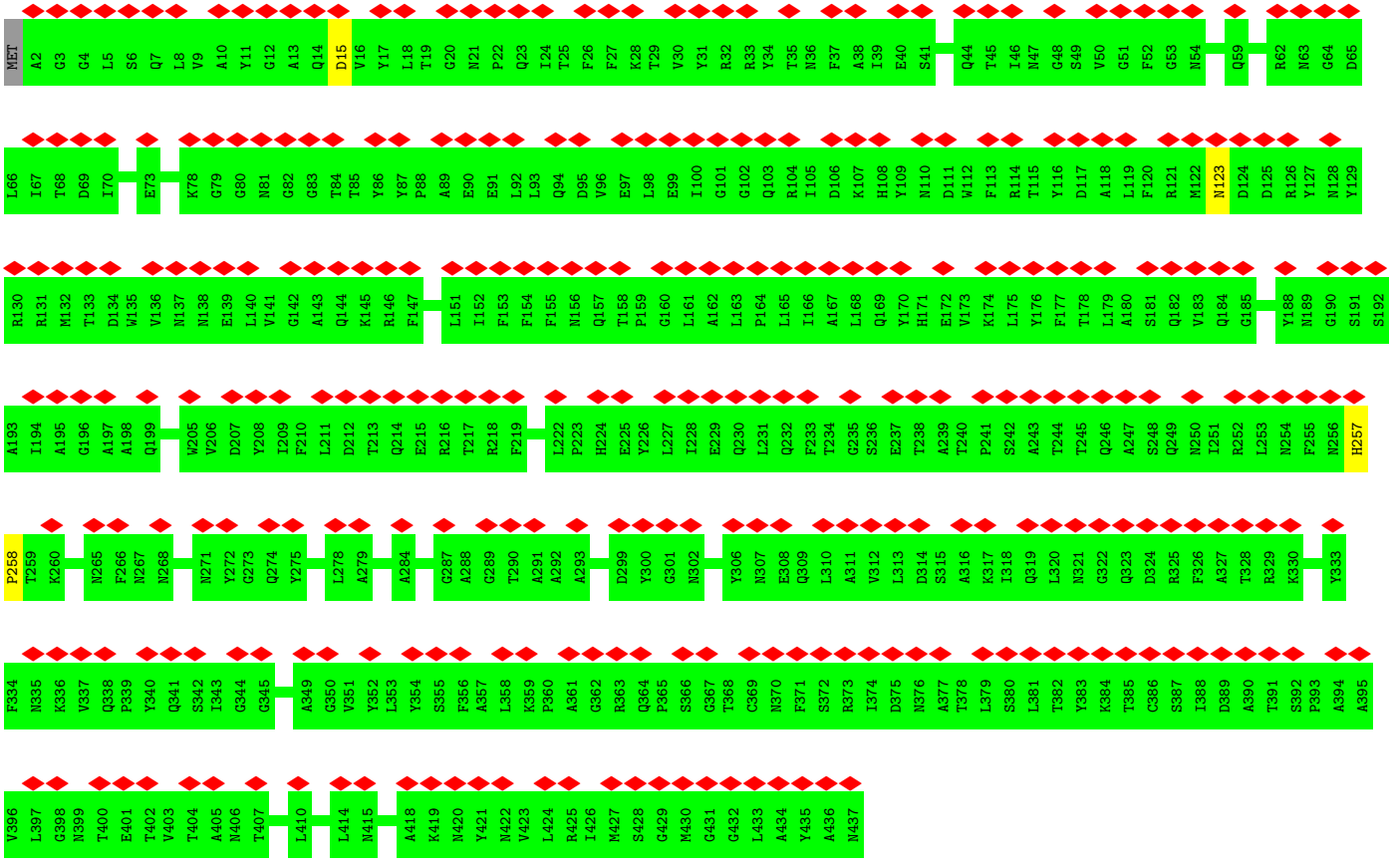




• Molecule 1: Major capsid protein (MCP)

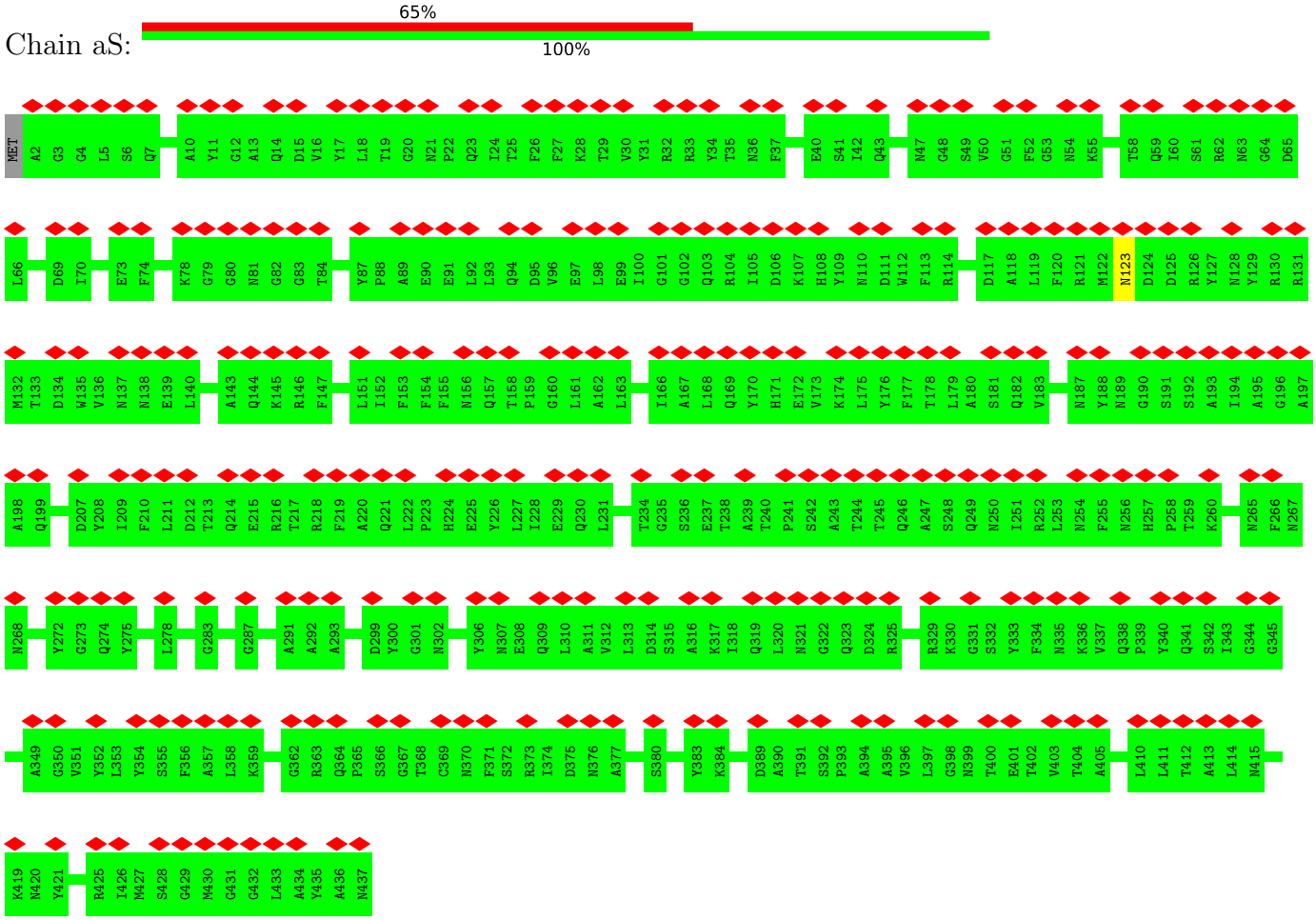
Chain aR:





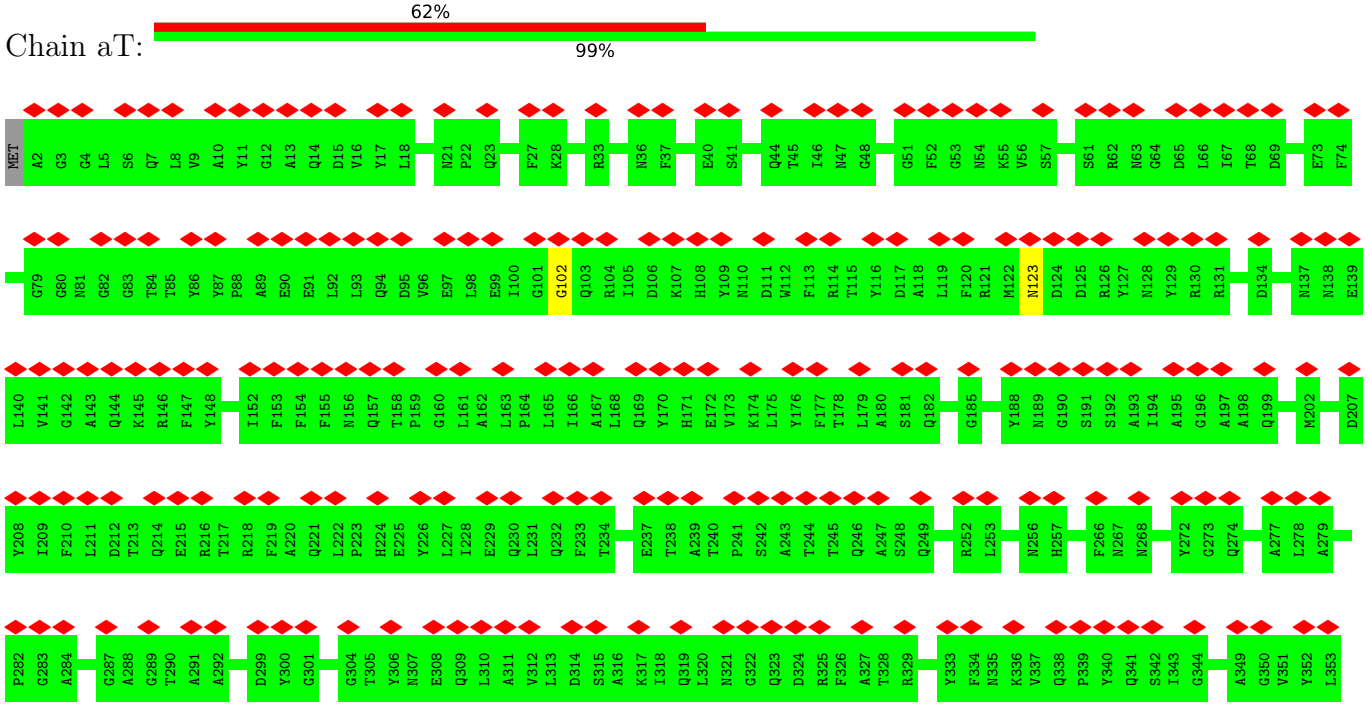
• Molecule 1: Major capsid protein (MCP)

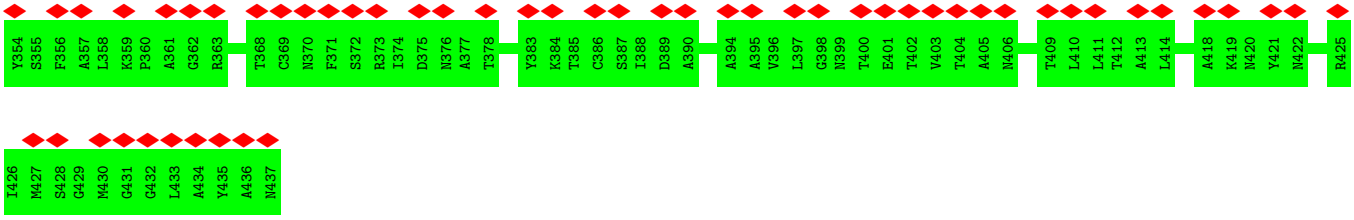
Chain aS:



• Molecule 1: Major capsid protein (MCP)

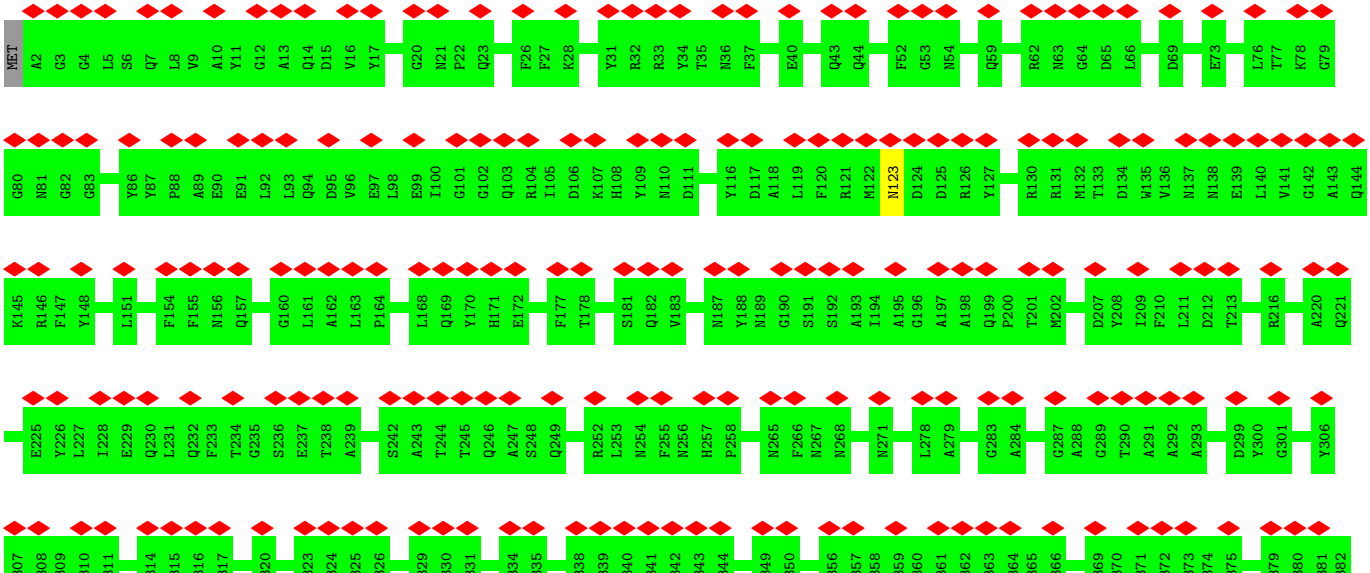
Chain aT:





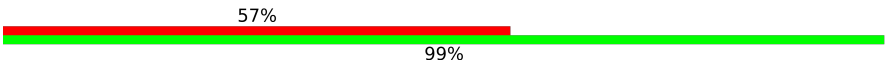
• Molecule 1: Major capsid protein (MCP)

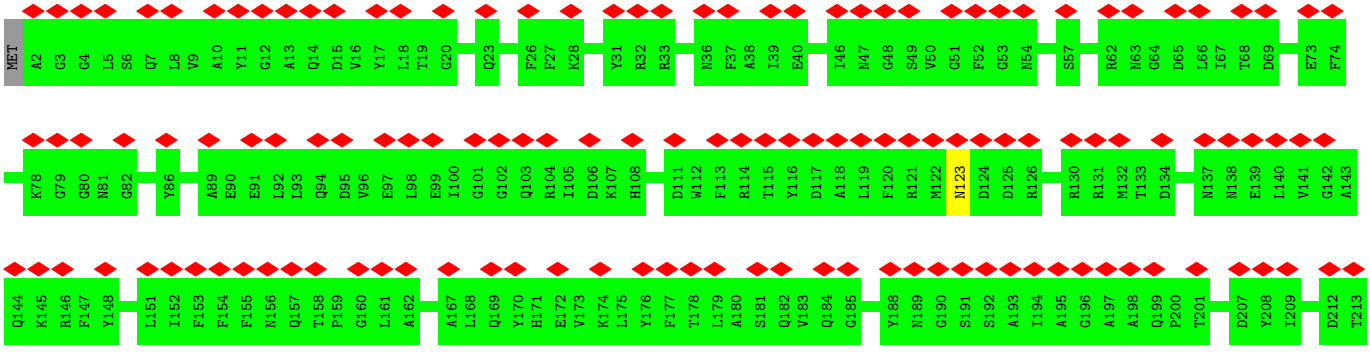
Chain aU:

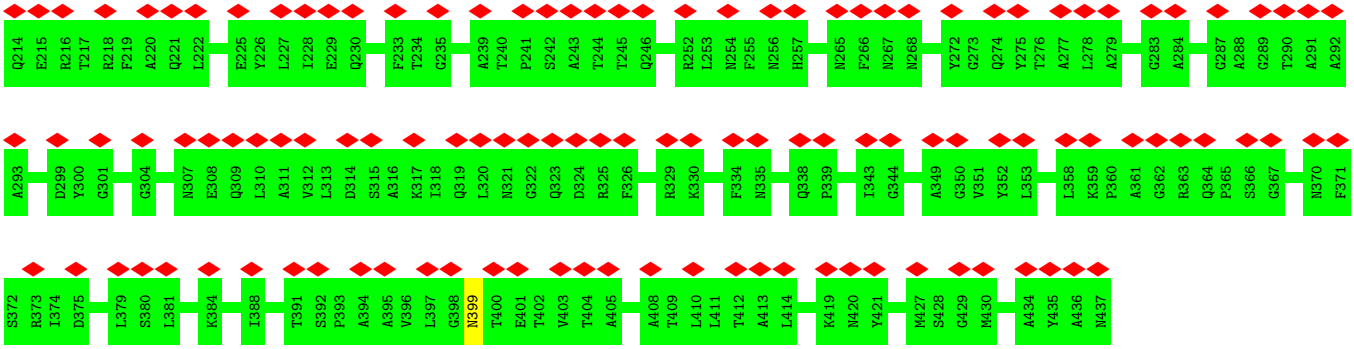


• Molecule 1: Major capsid protein (MCP)

Chain aV:

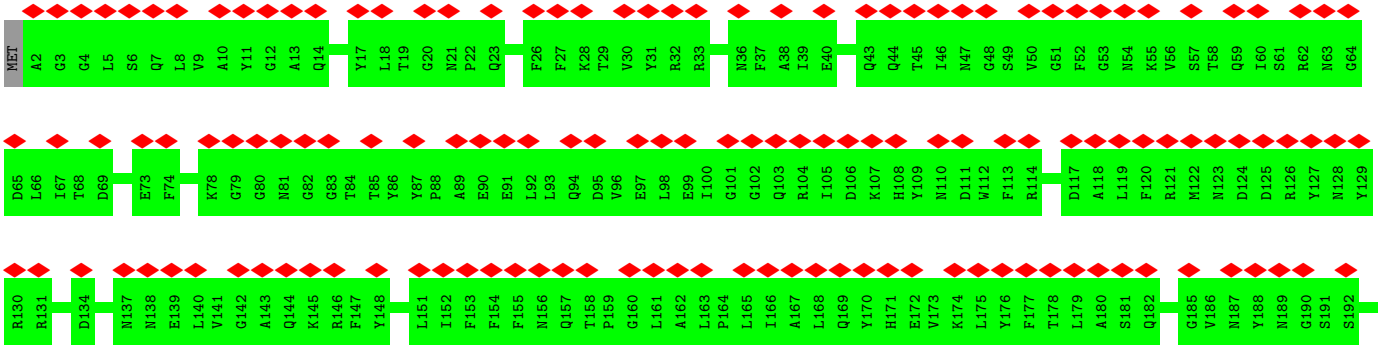






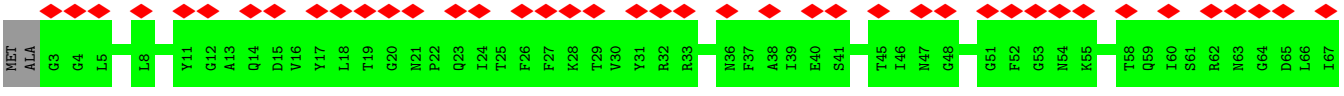
• Molecule 1: Major capsid protein (MCP)

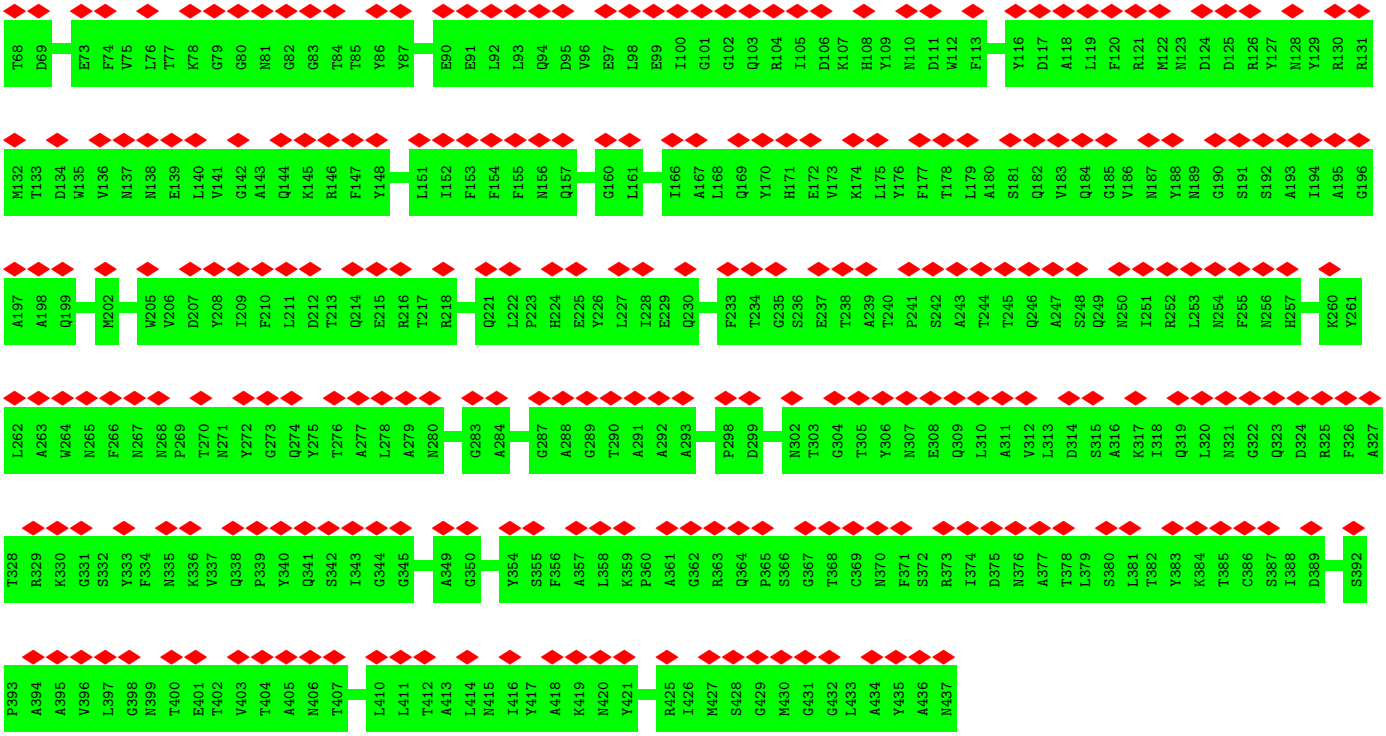
Chain aW:



• Molecule 1: Major capsid protein (MCP)

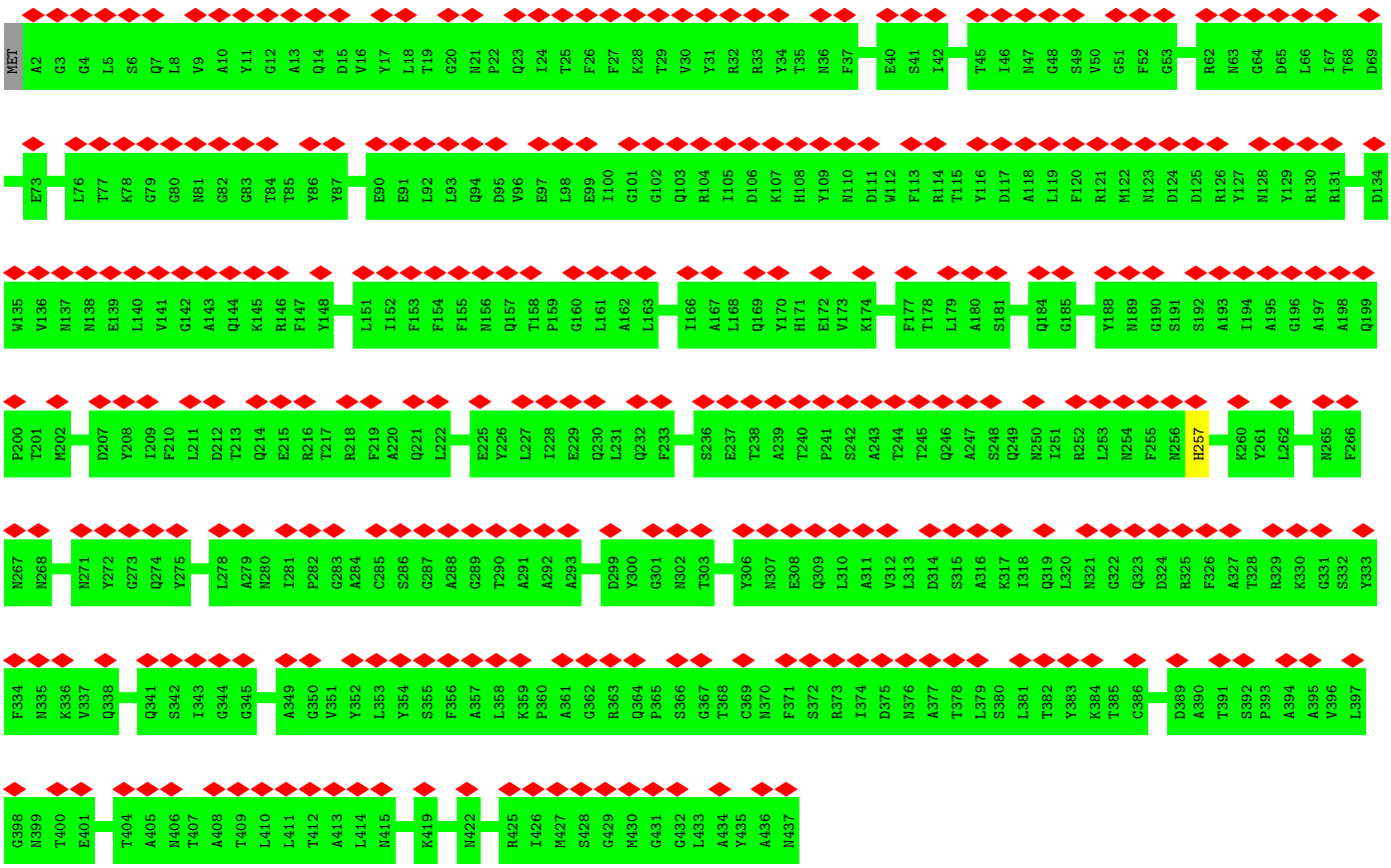
Chain aX:





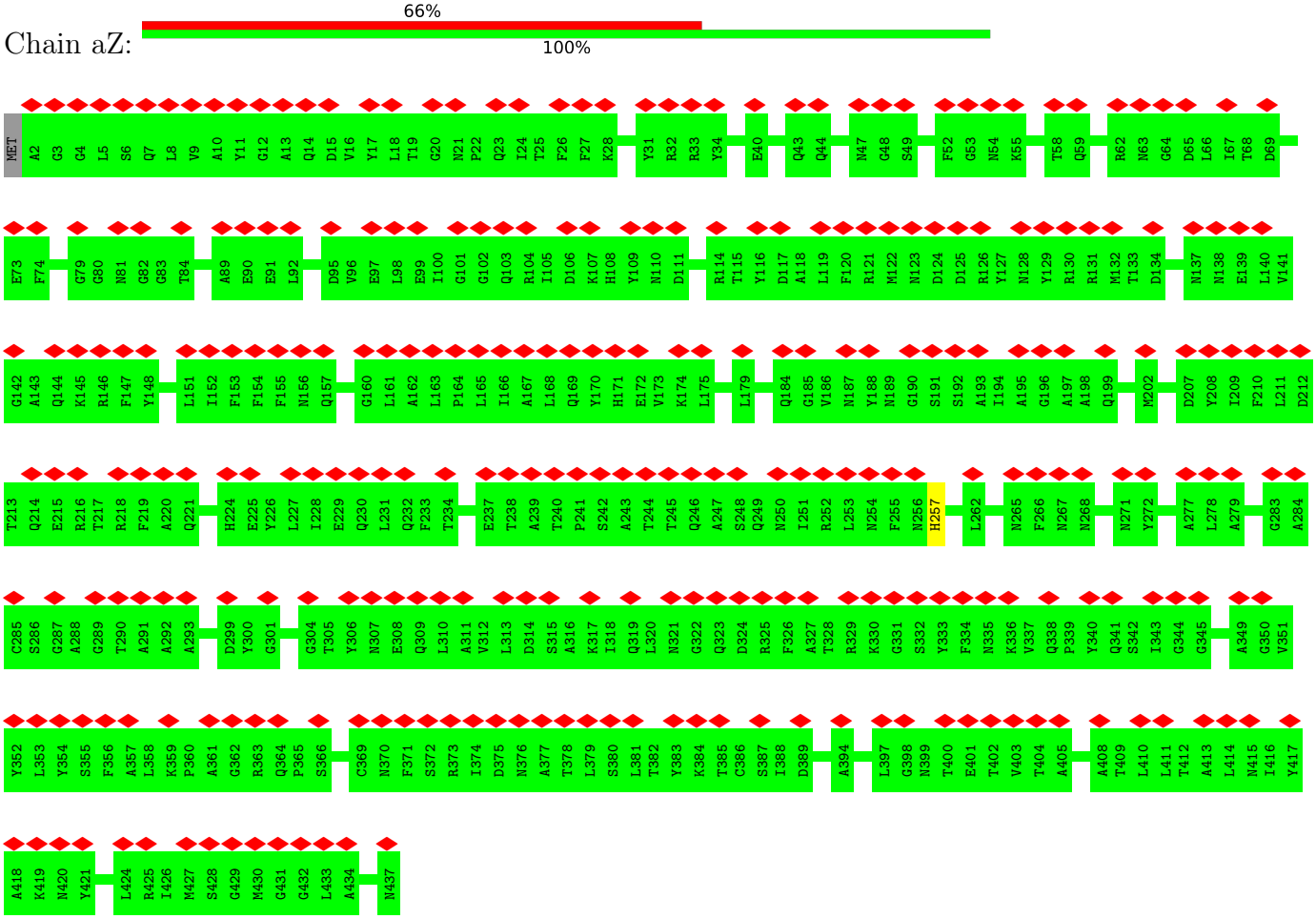
• Molecule 1: Major capsid protein (MCP)

Chain aY:



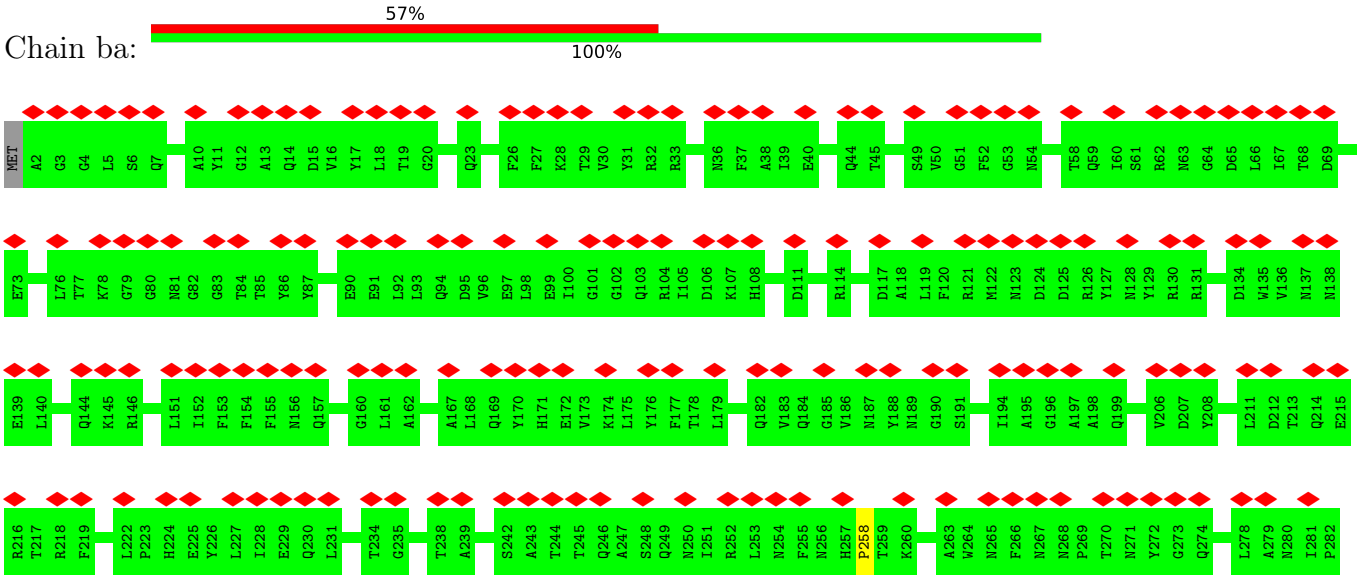
• Molecule 1: Major capsid protein (MCP)

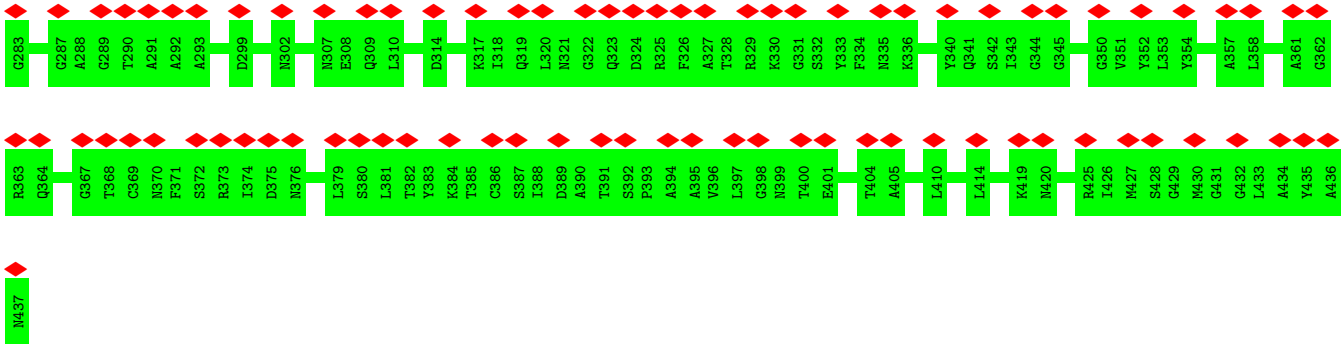
Chain aZ:



• Molecule 1: Major capsid protein (MCP)

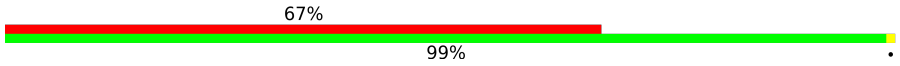
Chain ba:

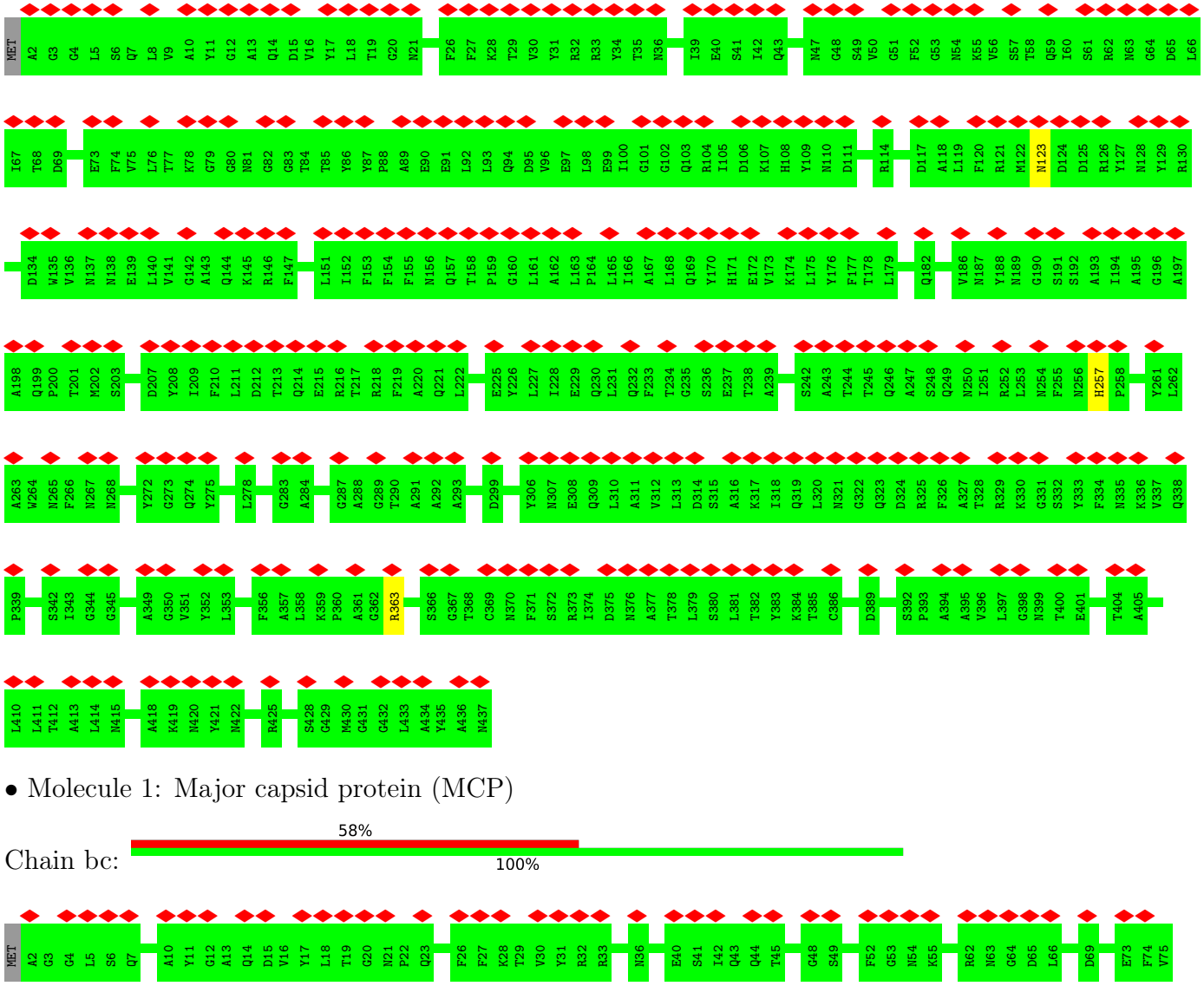




• Molecule 1: Major capsid protein (MCP)

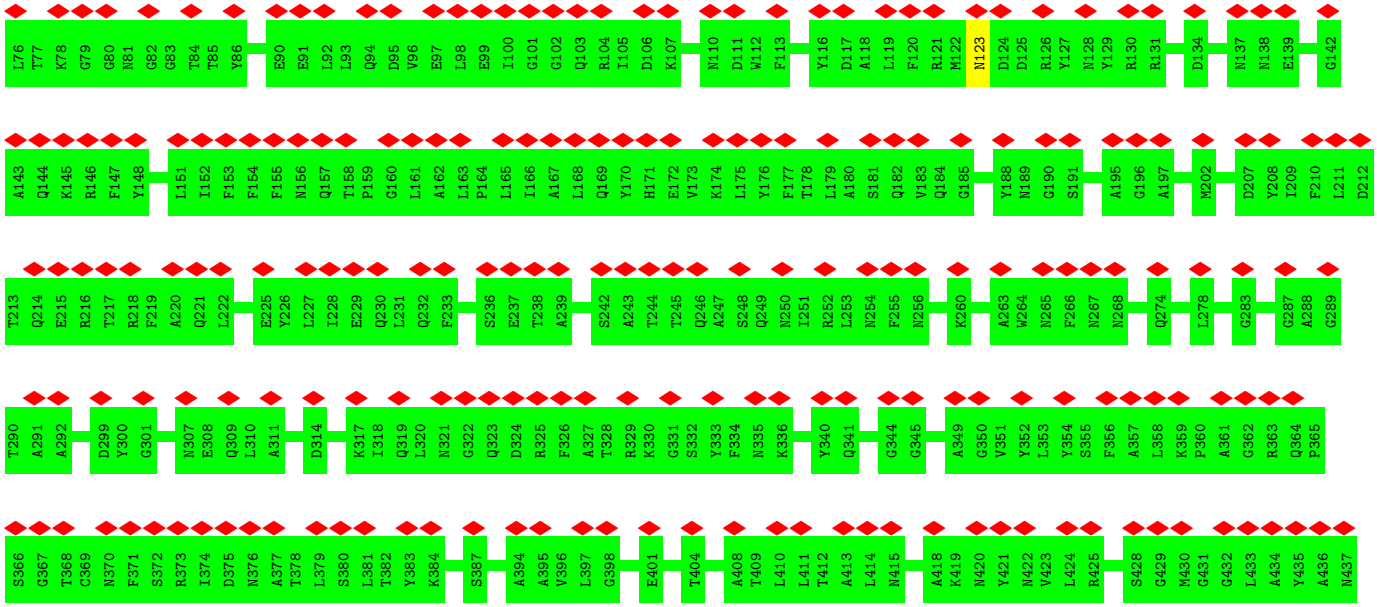
Chain bb:





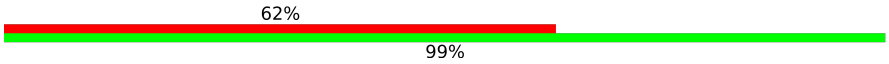
• Molecule 1: Major capsid protein (MCP)

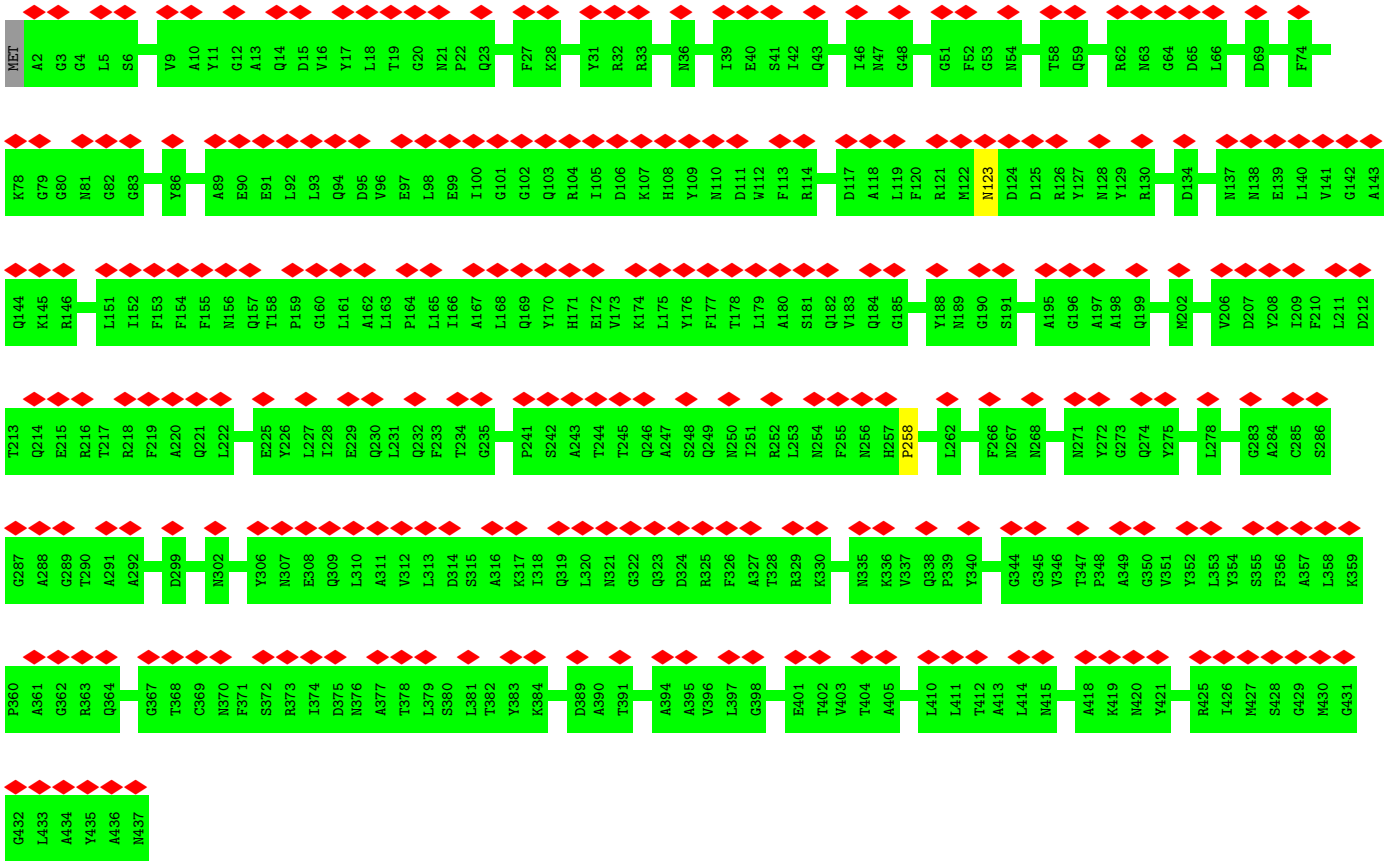
Chain bc:



• Molecule 1: Major capsid protein (MCP)

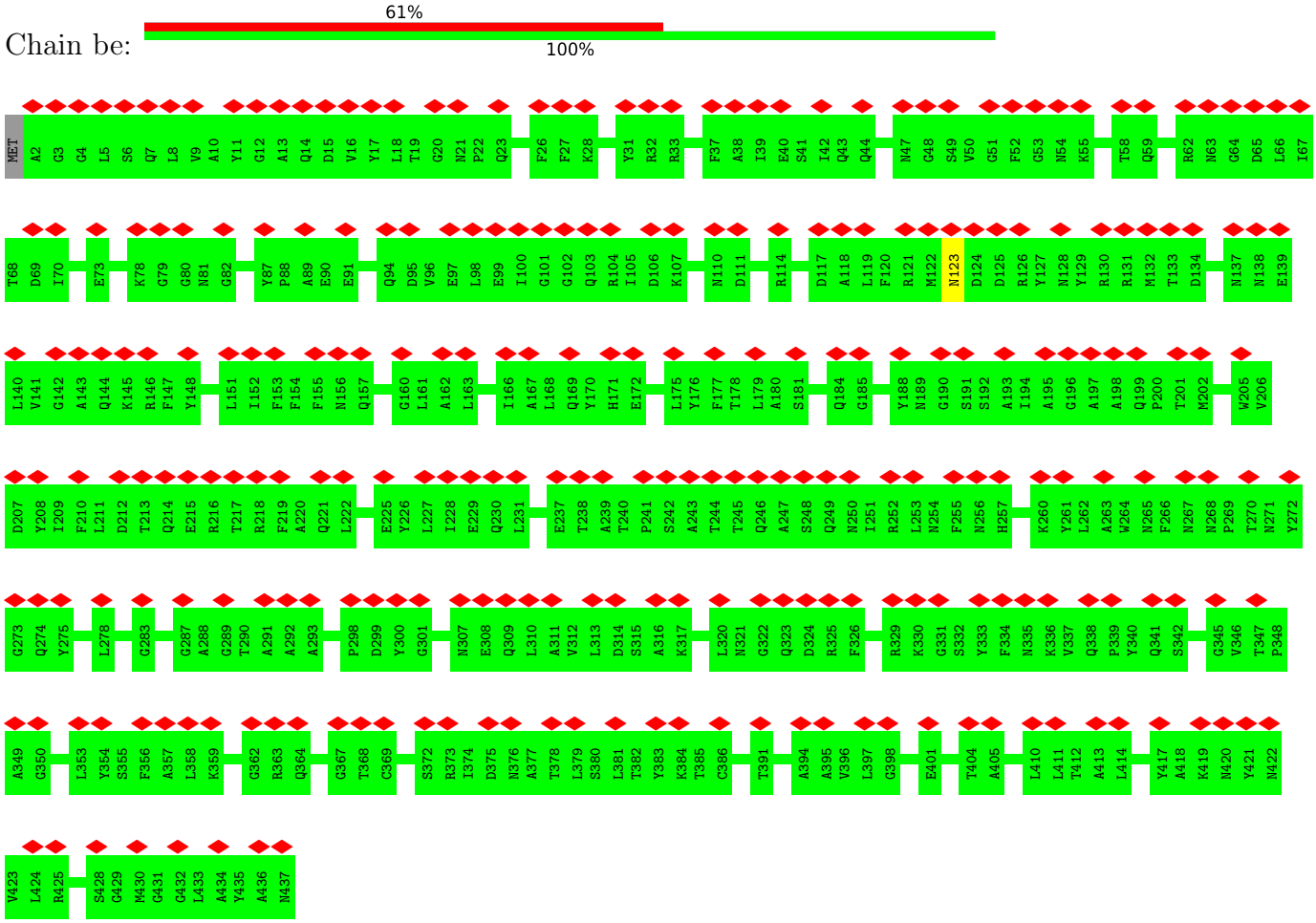
Chain bd:





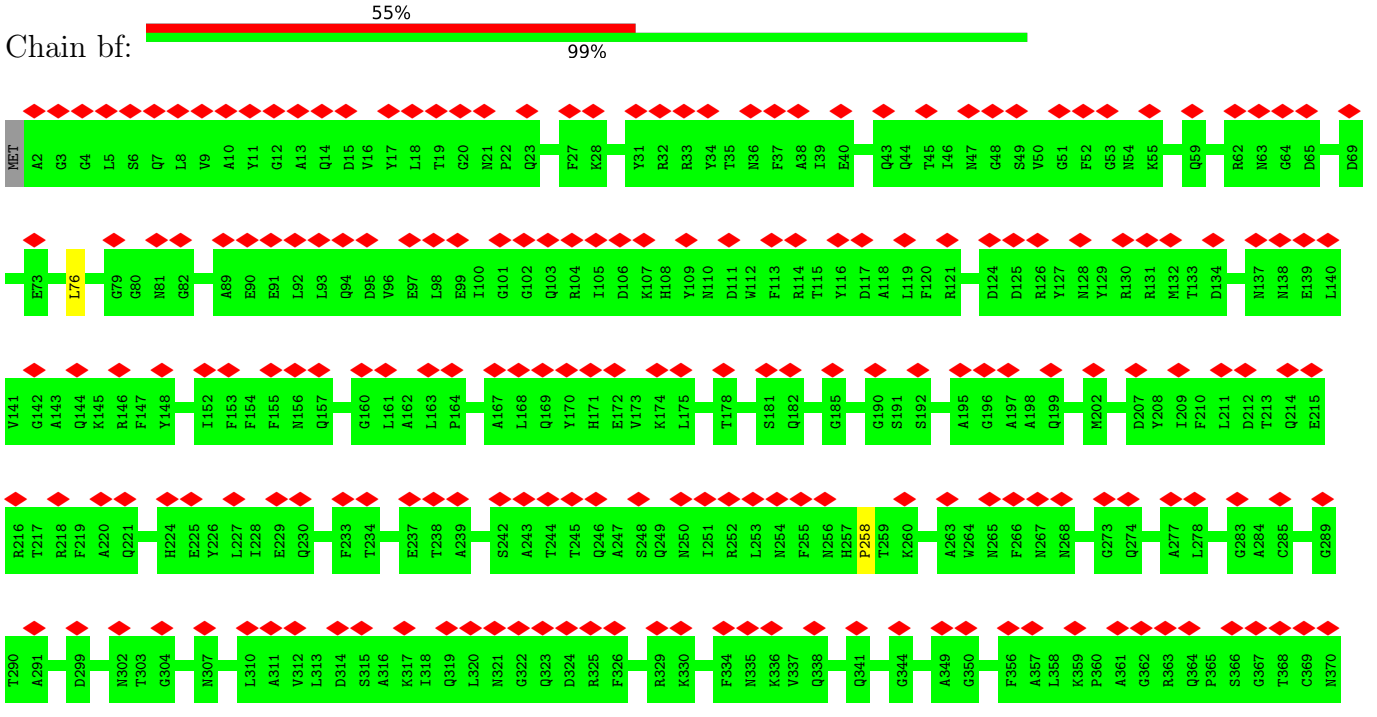
• Molecule 1: Major capsid protein (MCP)

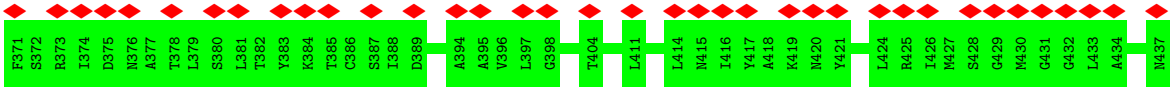
Chain be:



• Molecule 1: Major capsid protein (MCP)

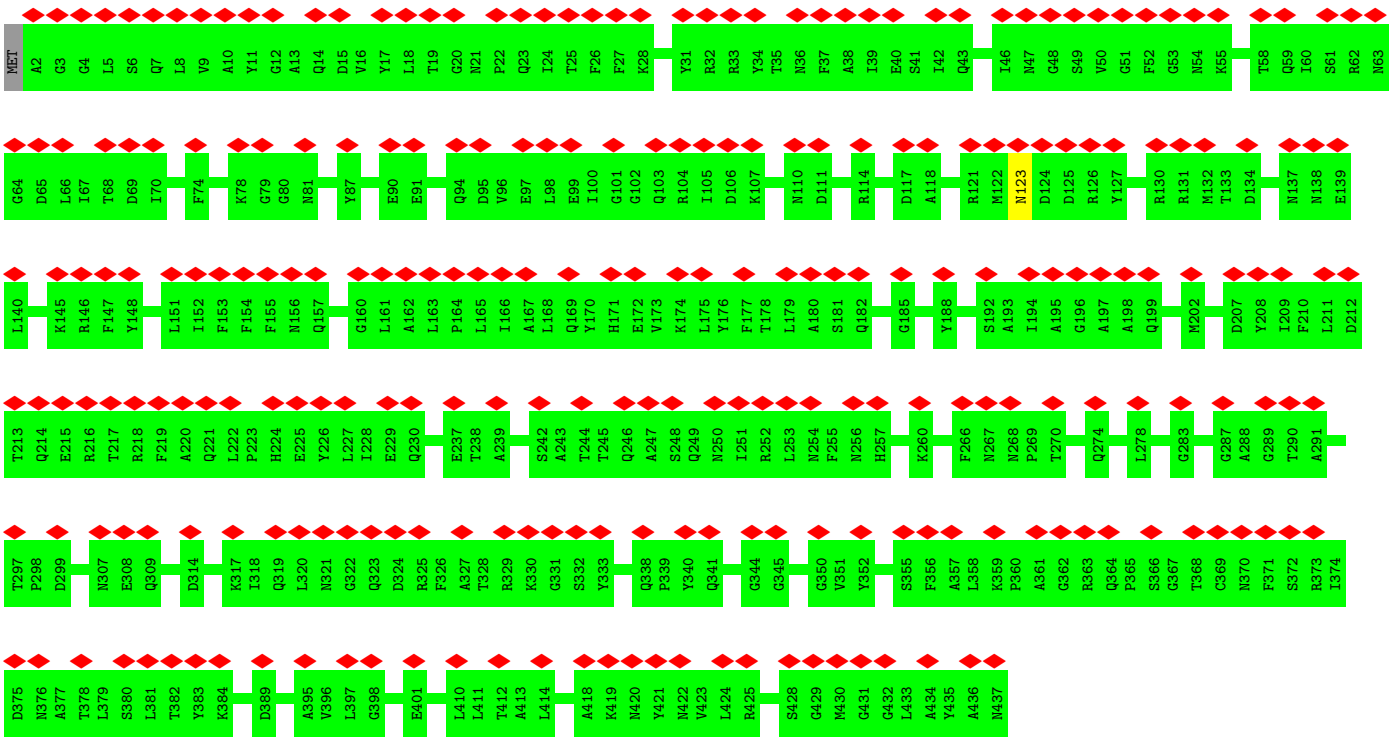
Chain bf:





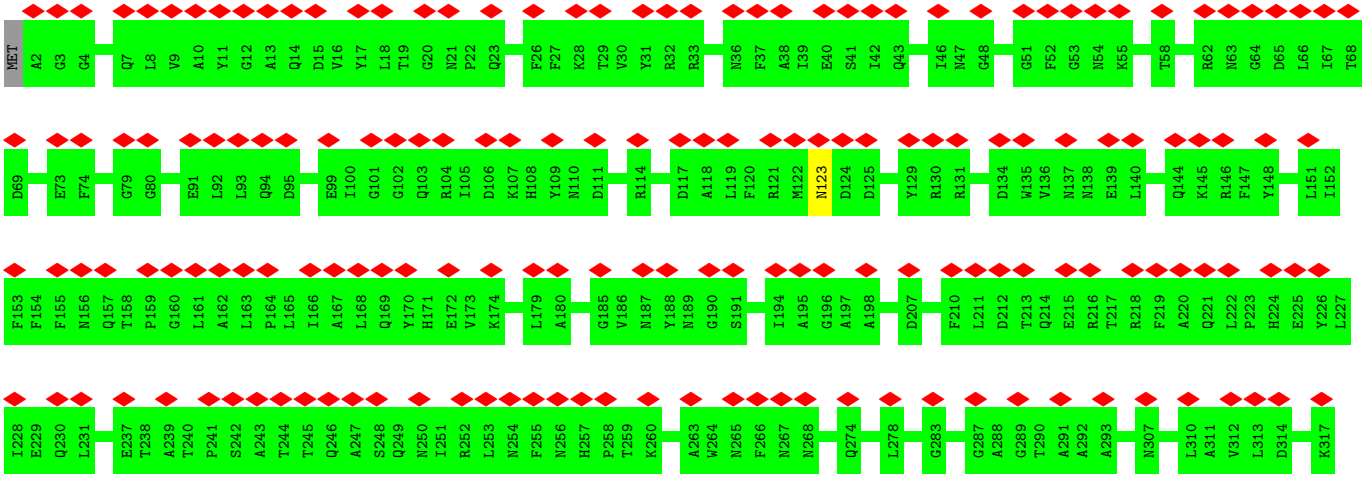
• Molecule 1: Major capsid protein (MCP)

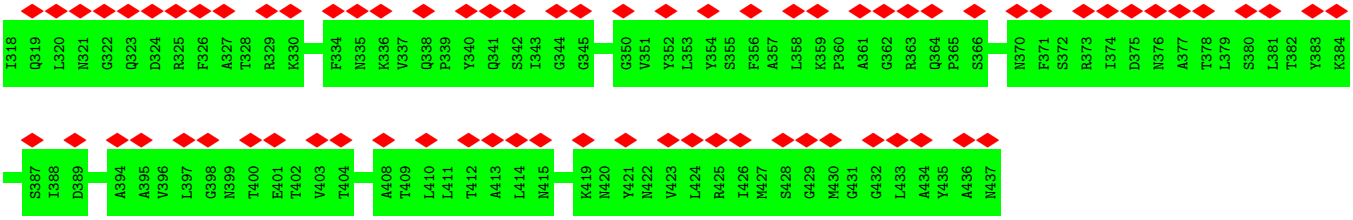
Chain bg:



• Molecule 1: Major capsid protein (MCP)

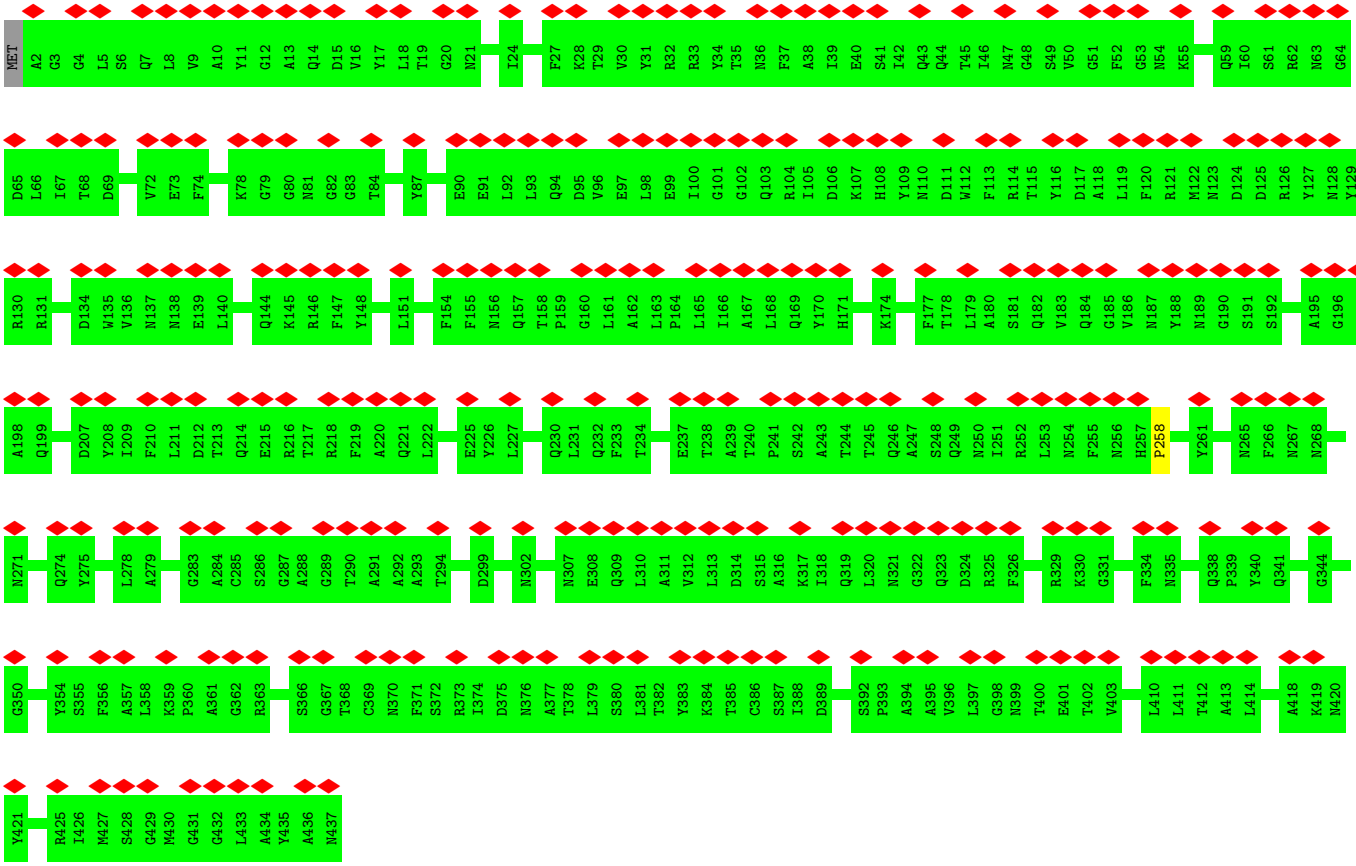
Chain bh:





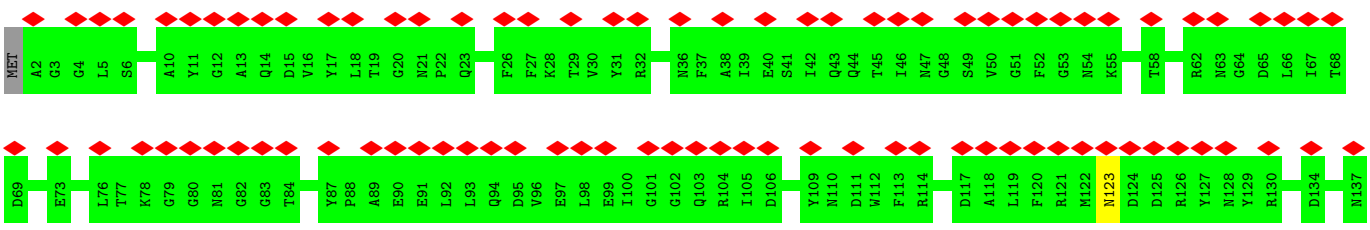
• Molecule 1: Major capsid protein (MCP)

Chain bi:



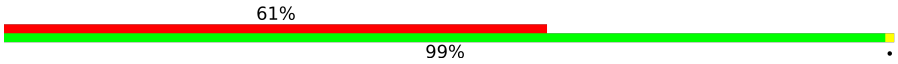
• Molecule 1: Major capsid protein (MCP)

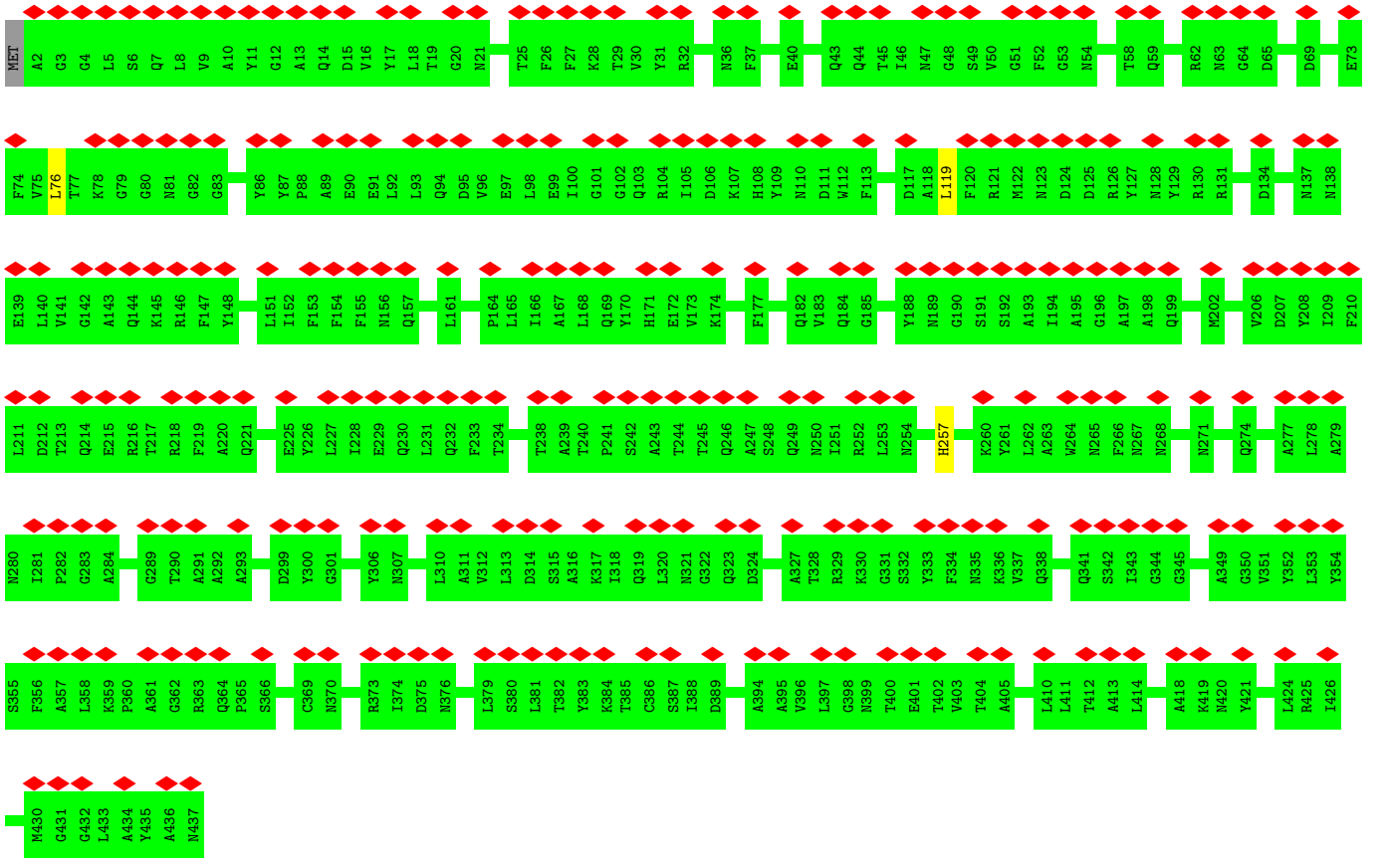
Chain bj:



• Molecule 1: Major capsid protein (MCP)

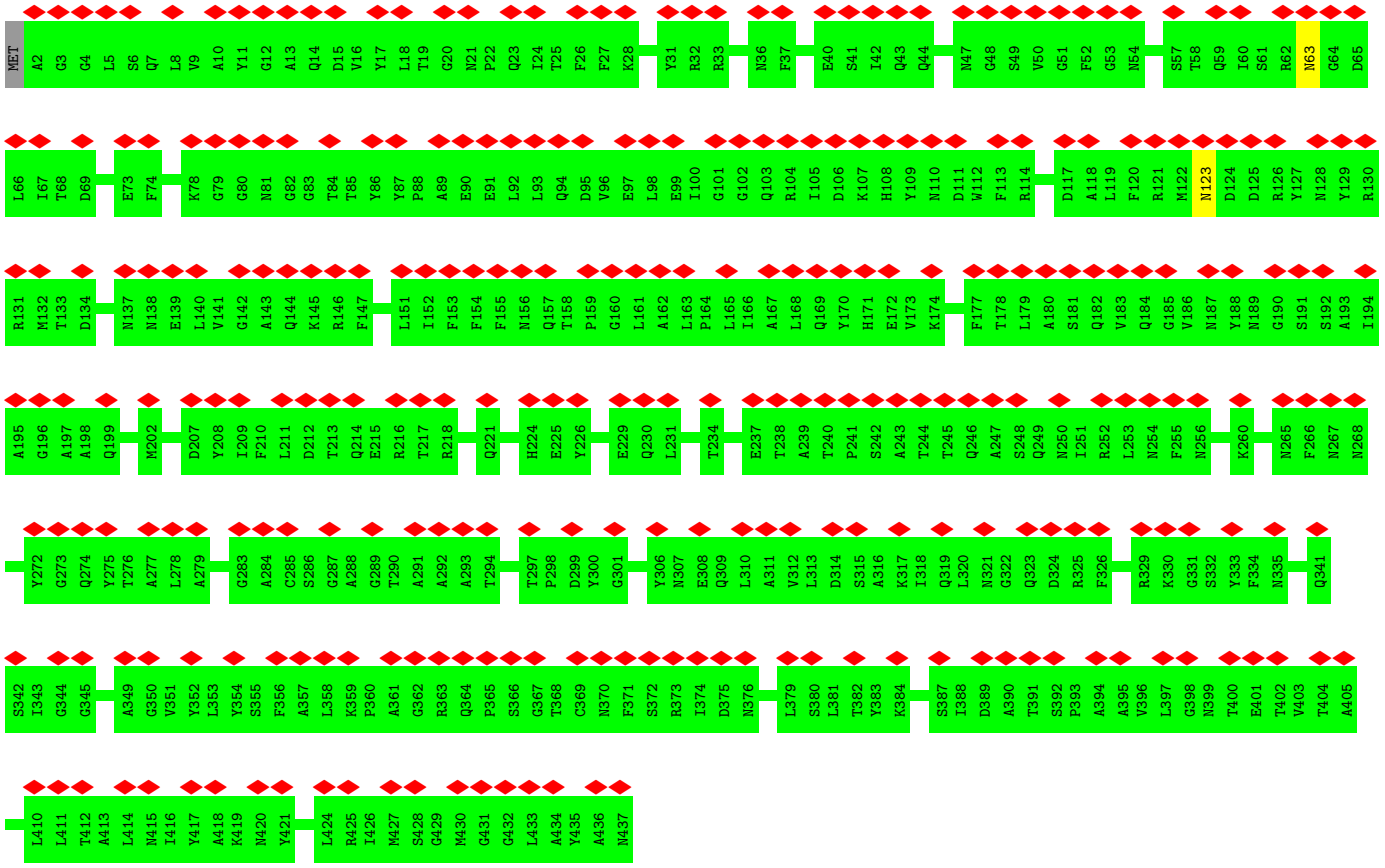
Chain bk:





• Molecule 1: Major capsid protein (MCP)

Chain bl:



• Molecule 1: Major capsid protein (MCP)

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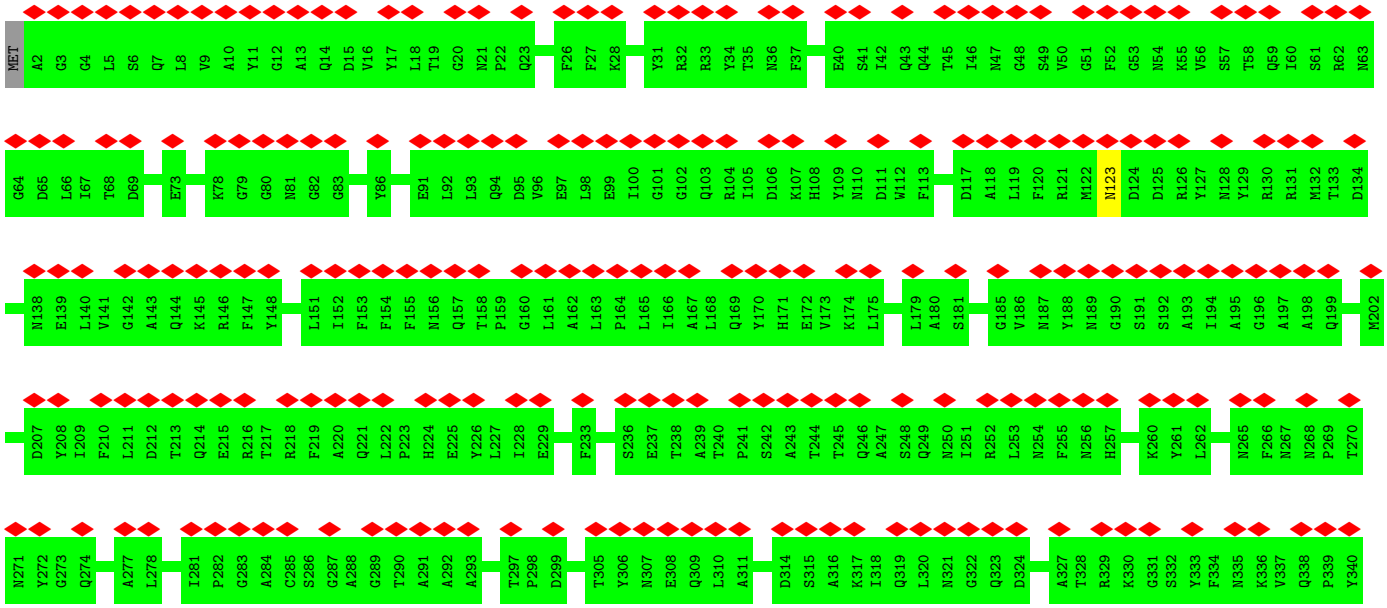
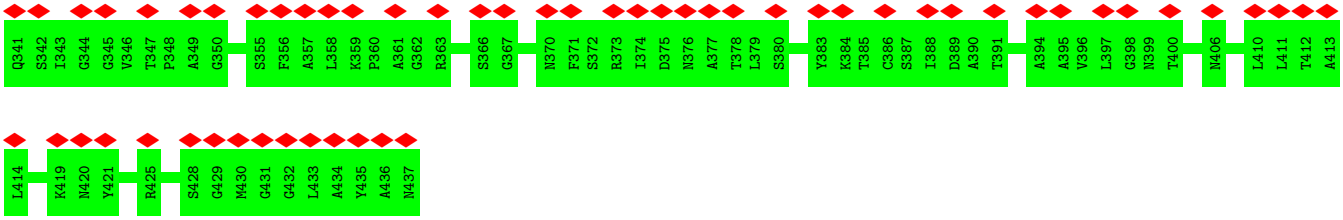
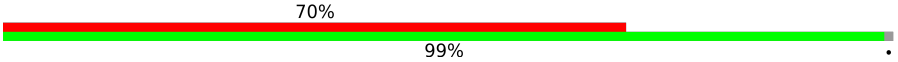




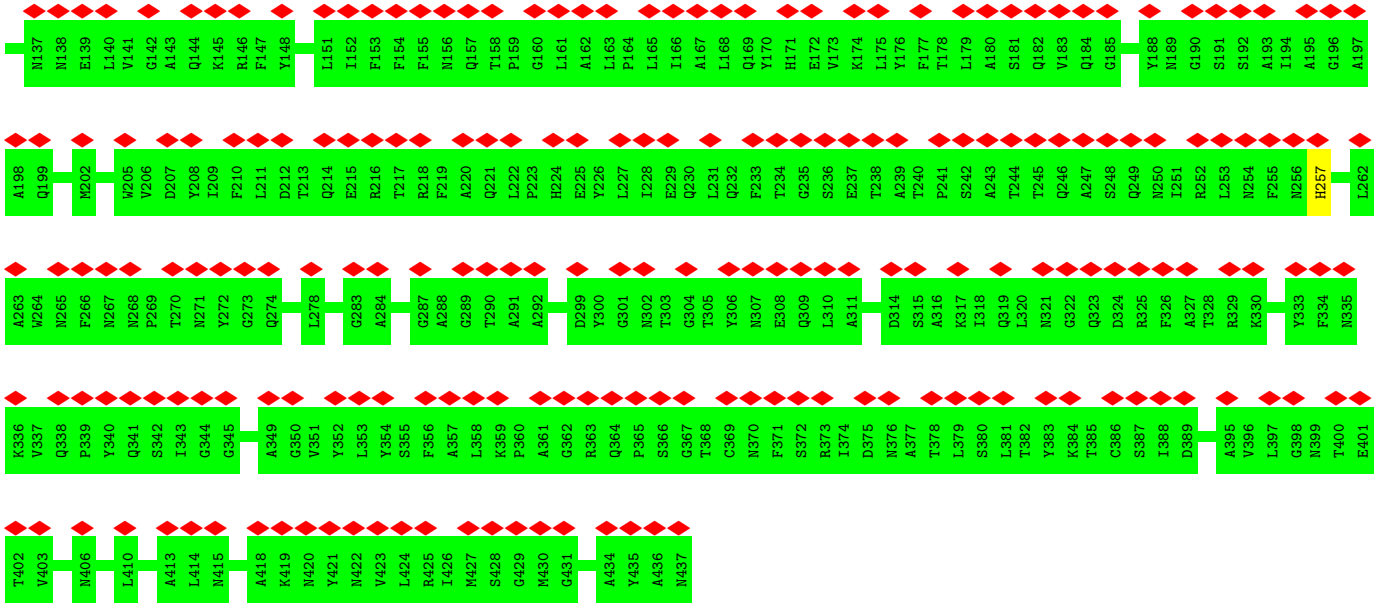
• Molecule 1: Major capsid protein (MCP)

Chain bn:



• Molecule 1: Major capsid protein (MCP)

Chain bo:



• Molecule 1: Major capsid protein (MCP)

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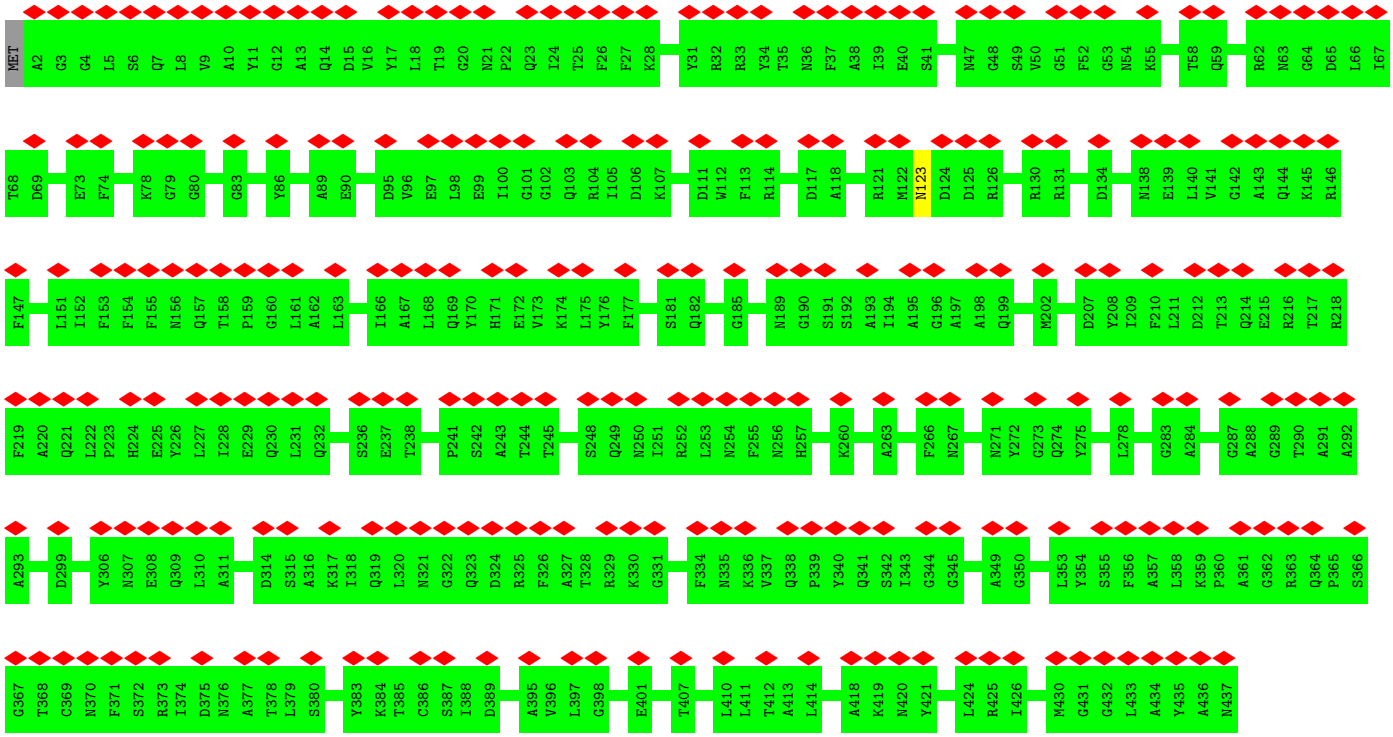
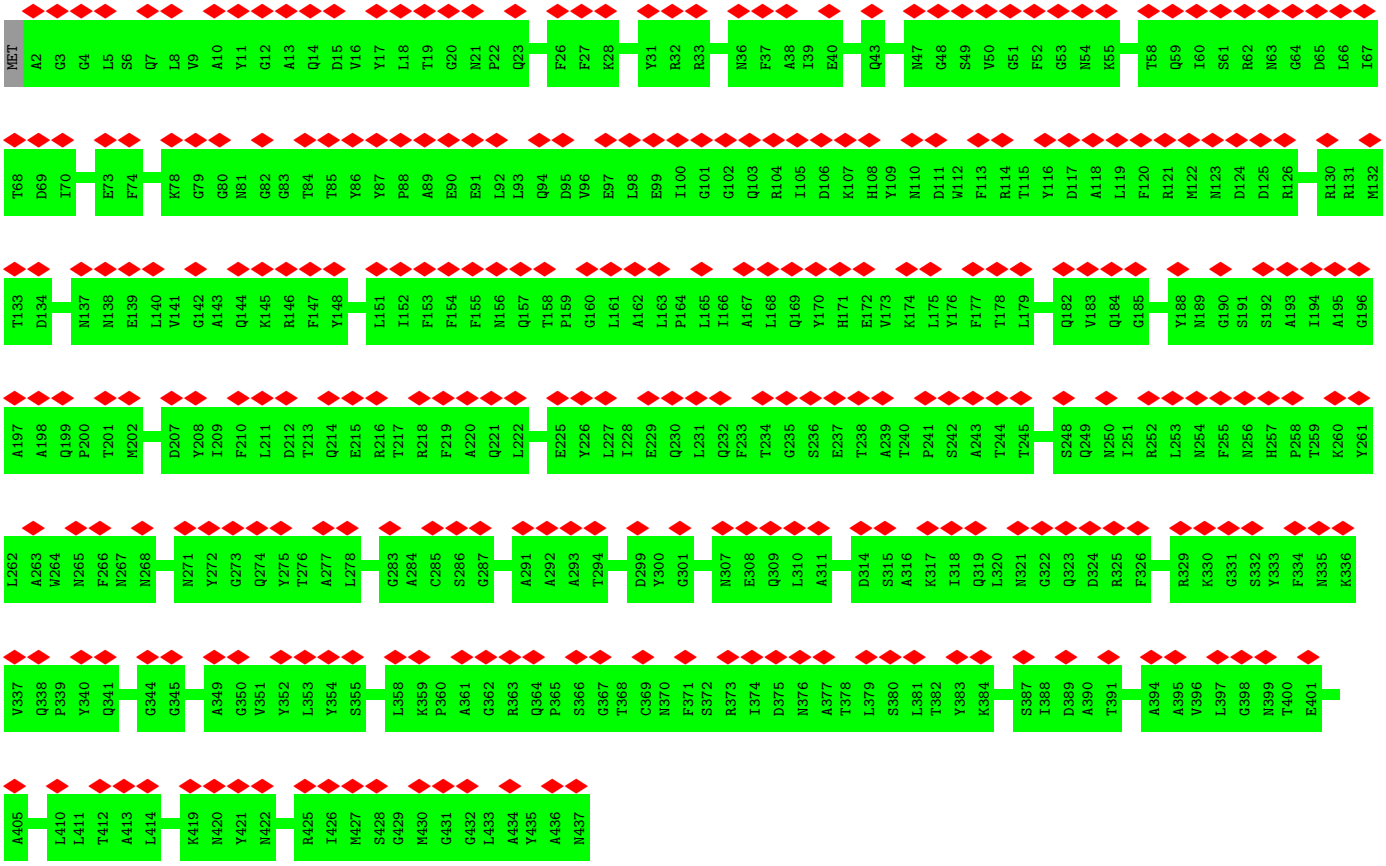


• Molecule 1: Major capsid protein (MCP)

Chain bq:



• Molecule 1: Major capsid protein (MCP)

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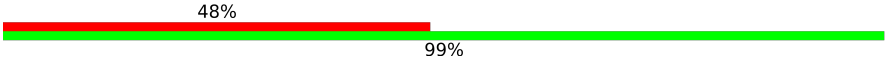
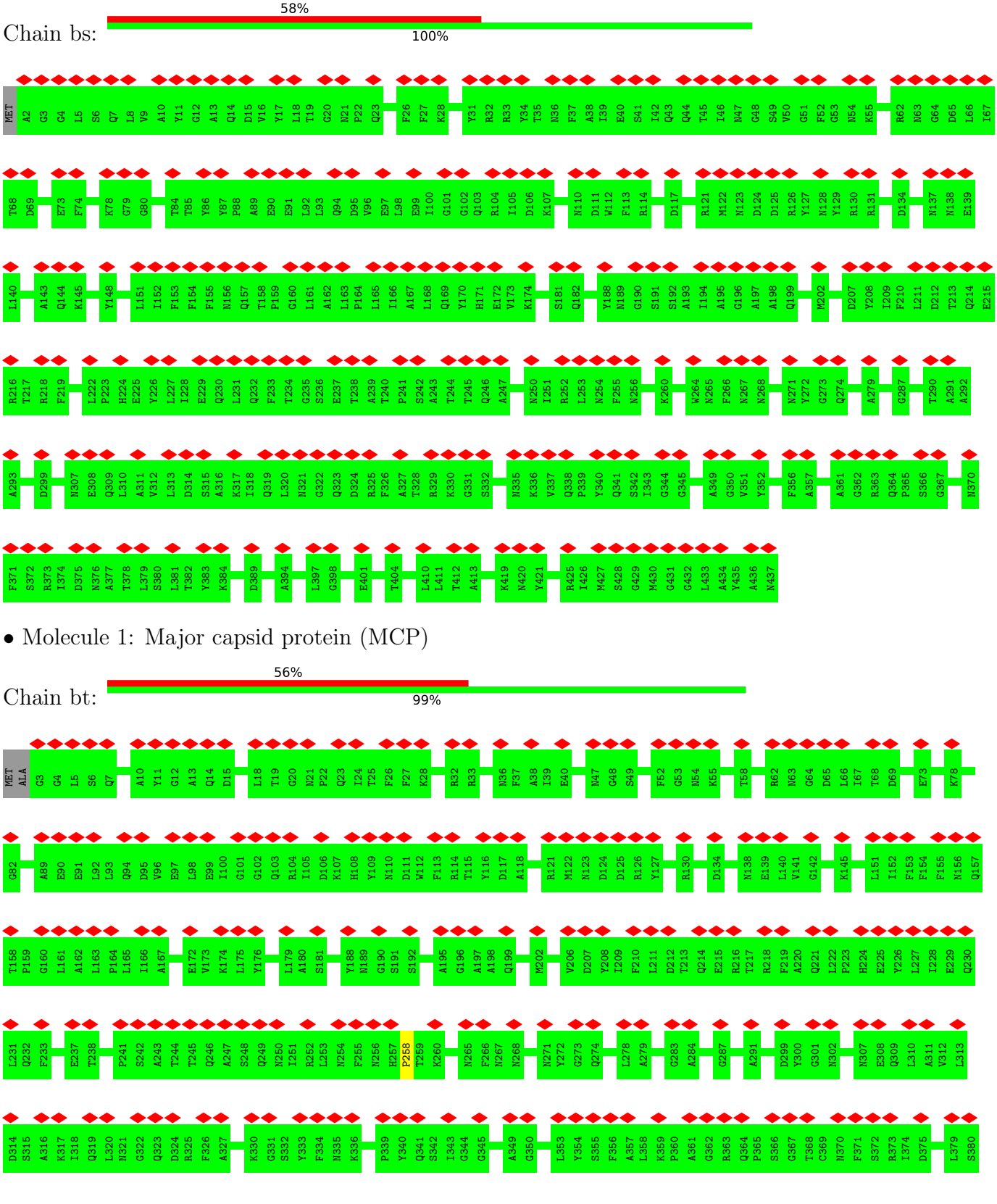


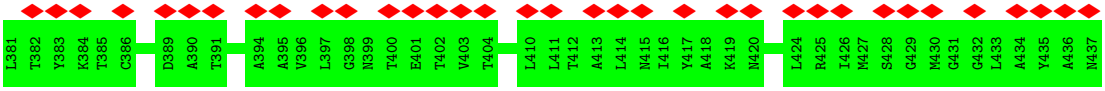
• Molecule 1: Major capsid protein (MCP)

Chain bs:



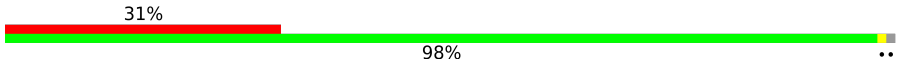
• Molecule 1: Major capsid protein (MCP)

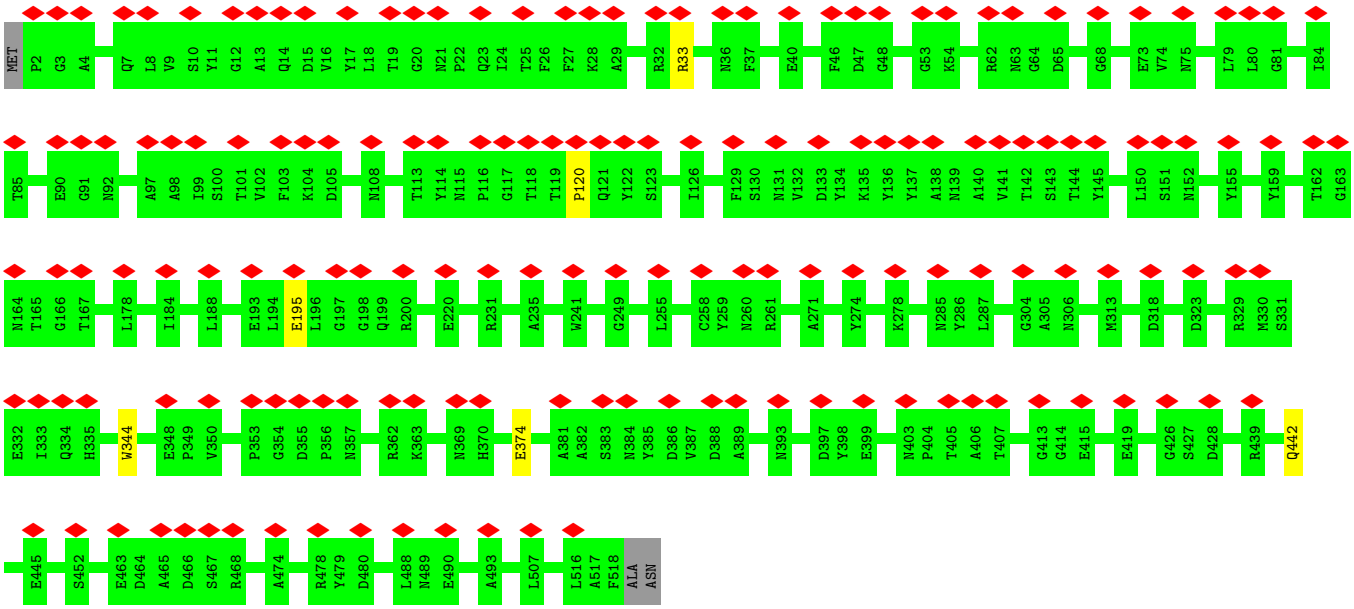
Chain bt:



• Molecule 2: MCPv1

Chain bu:





• Molecule 2: MCPv1

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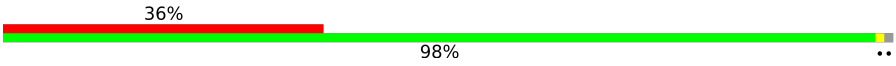
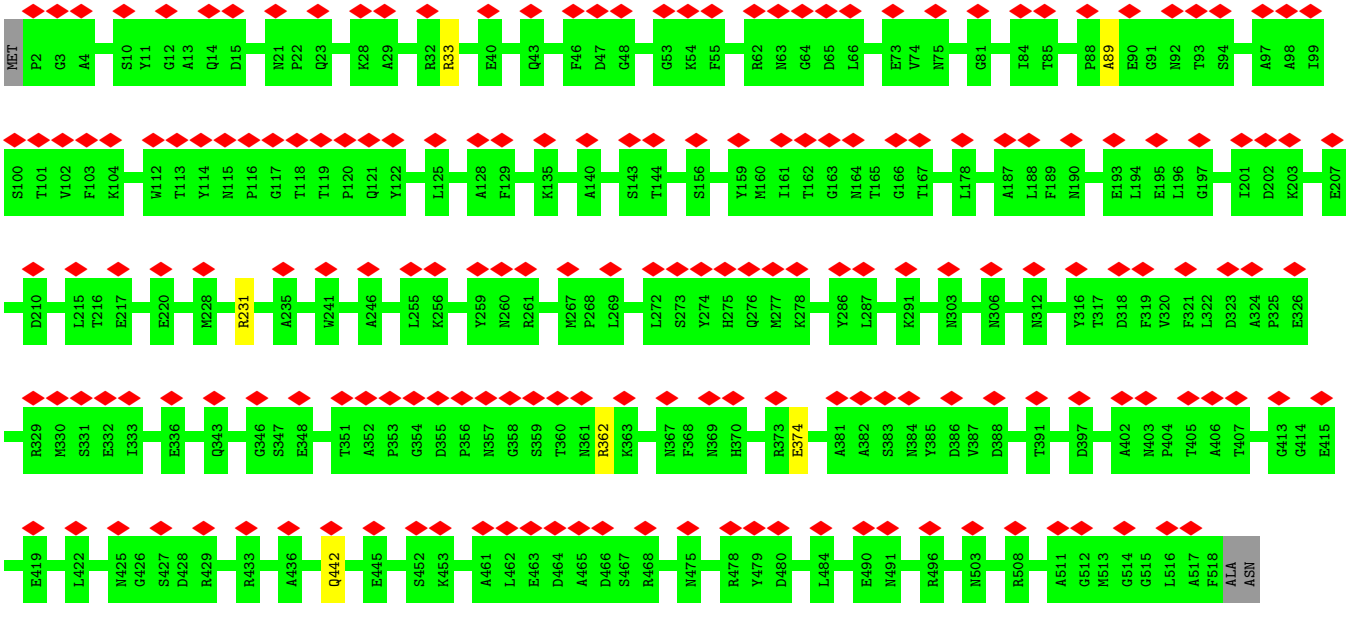
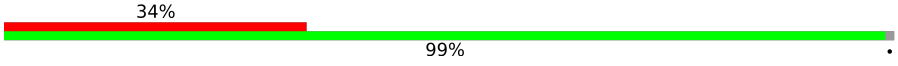
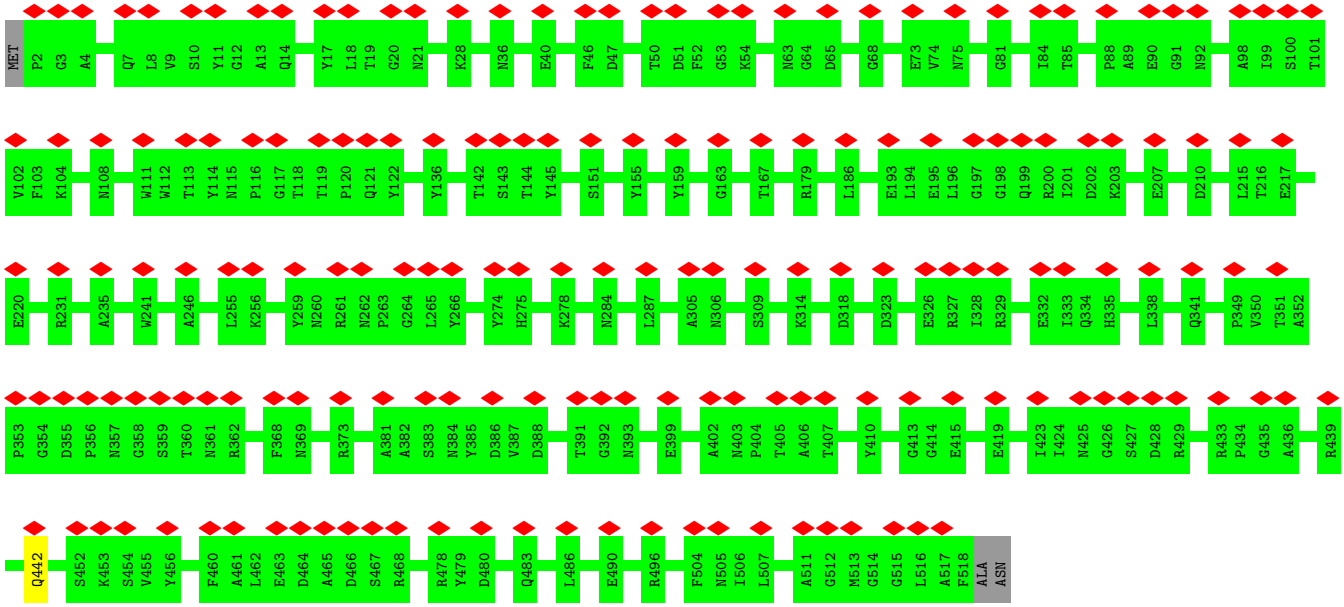




• Molecule 2: MCPv1

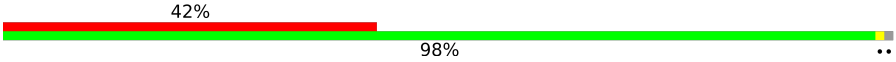
Chain bw:

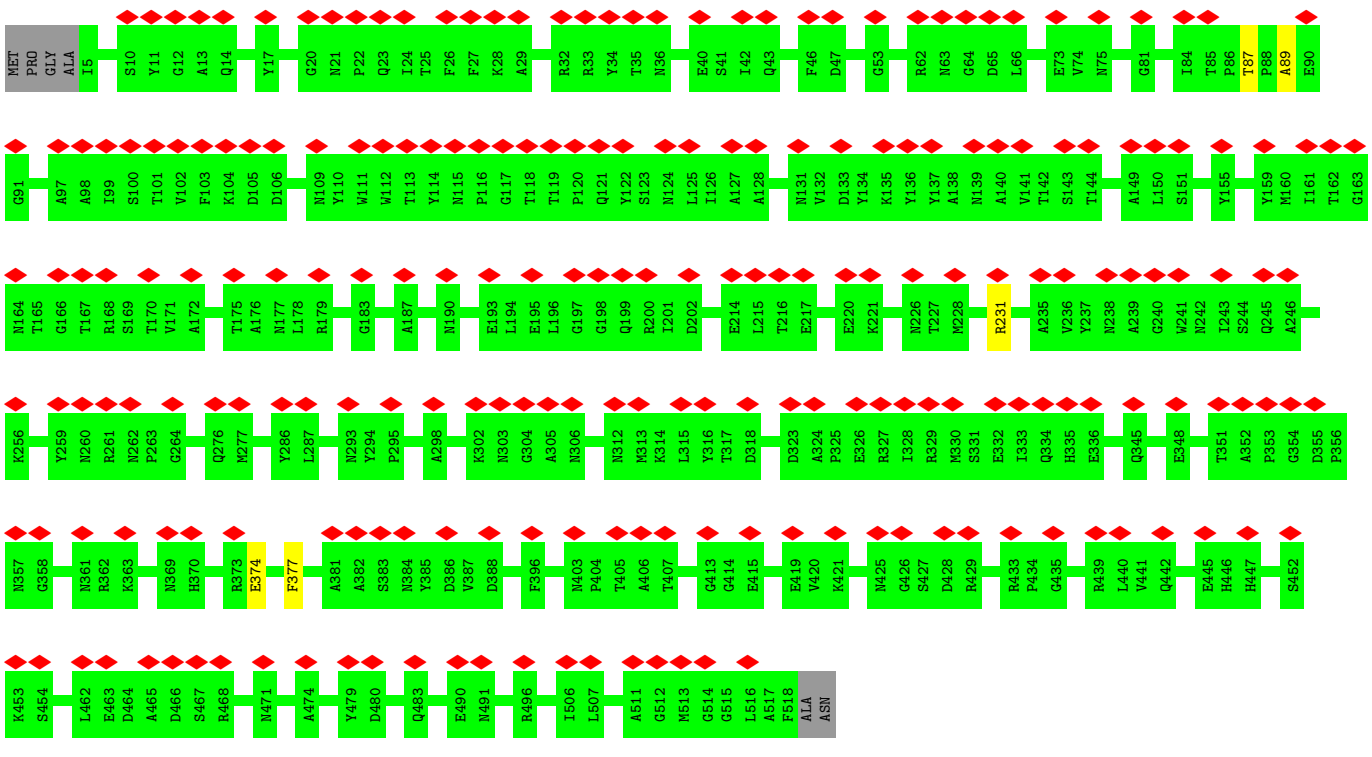




• Molecule 2: MCPv1

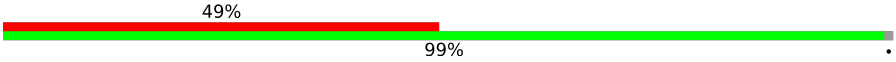
Chain bx:

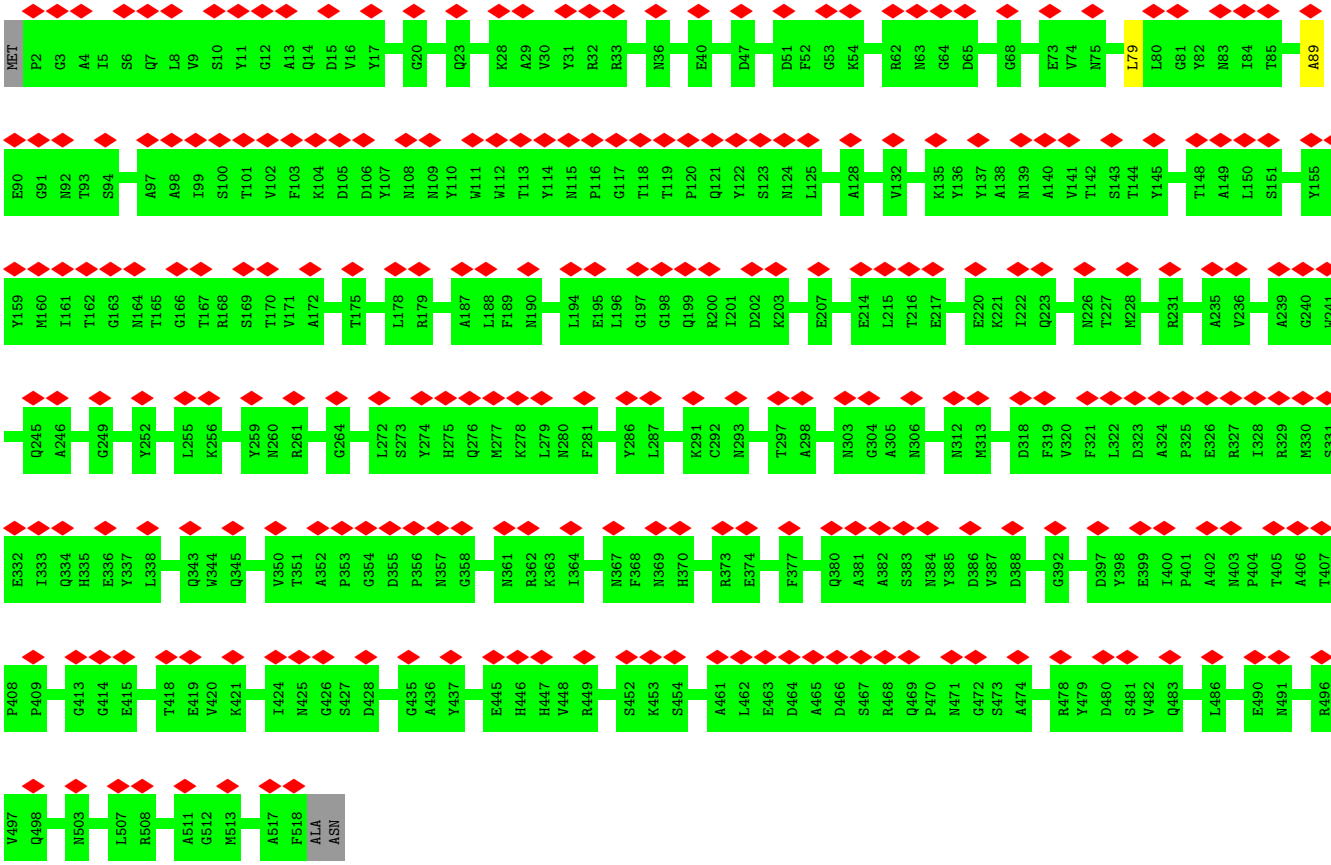




• Molecule 2: MCPv1

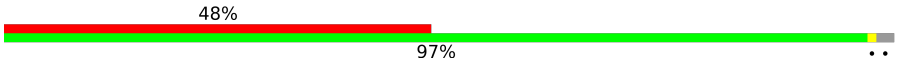
Chain by:

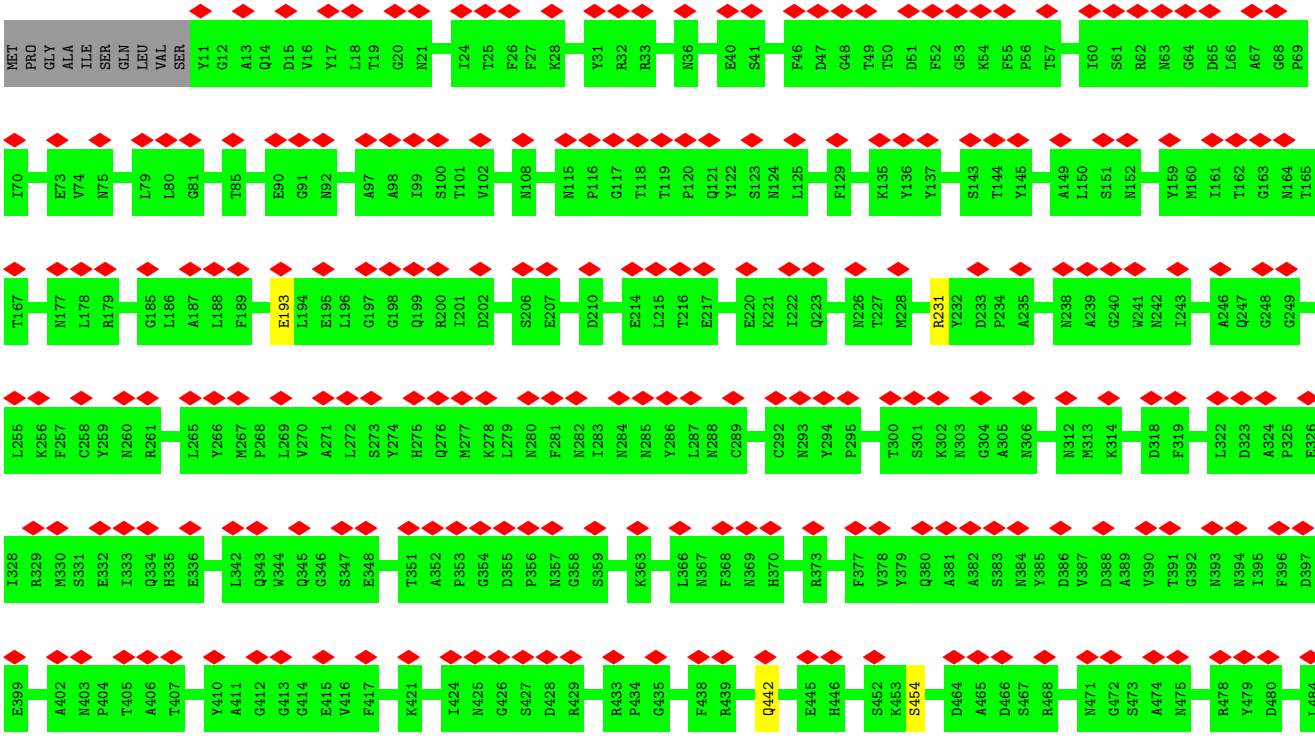


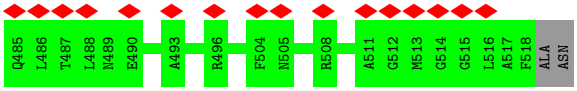


- Molecule 2: MCPv1

Chain bz:

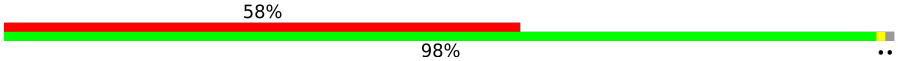


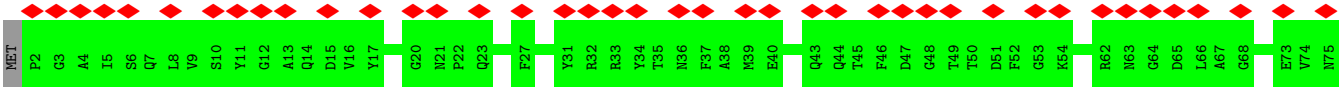


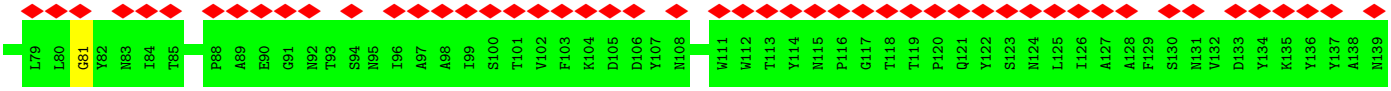


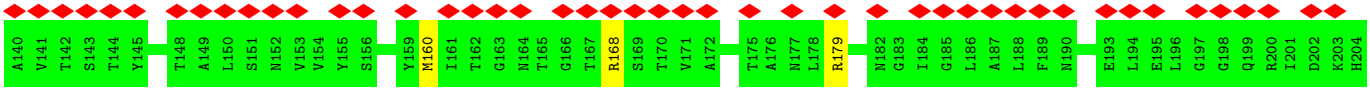
• Molecule 2: MCPv1

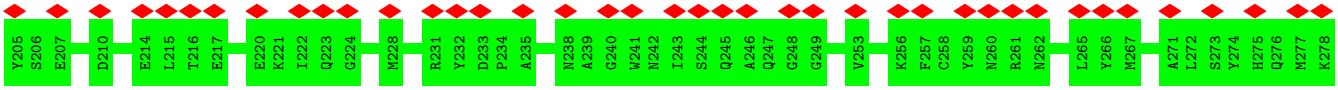
Chain bA:

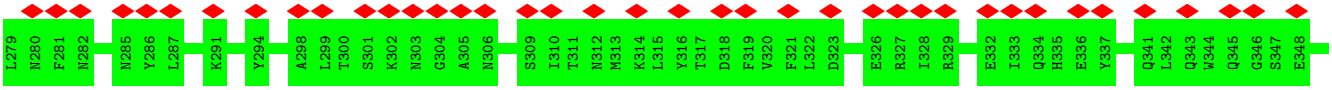


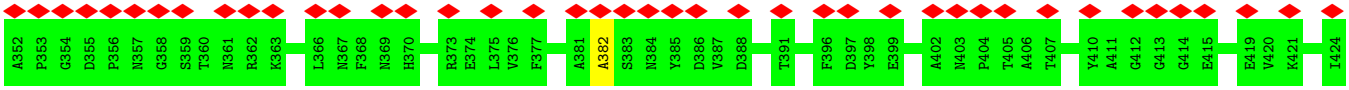


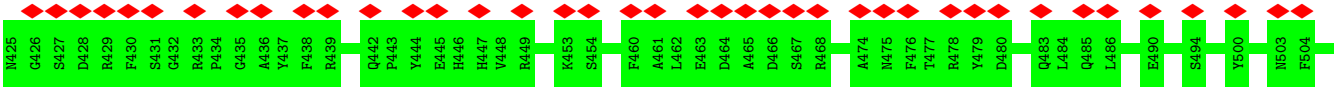


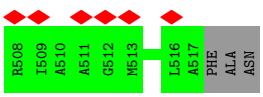






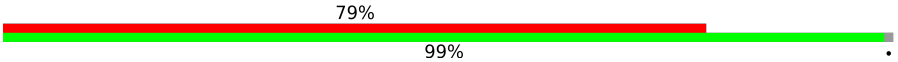


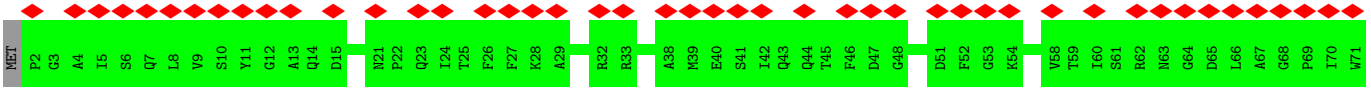


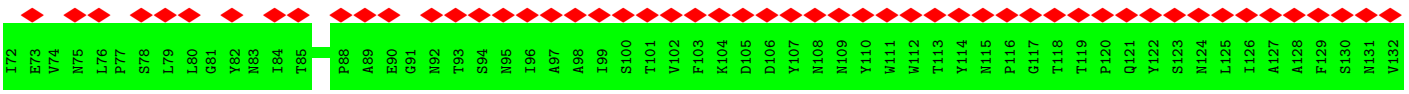


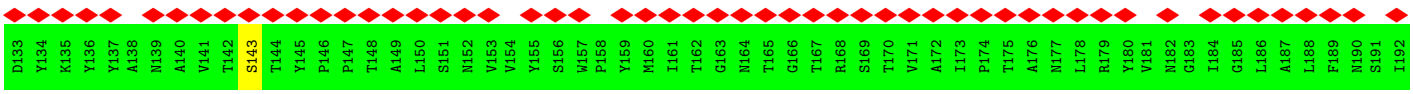
• Molecule 2: MCPv1

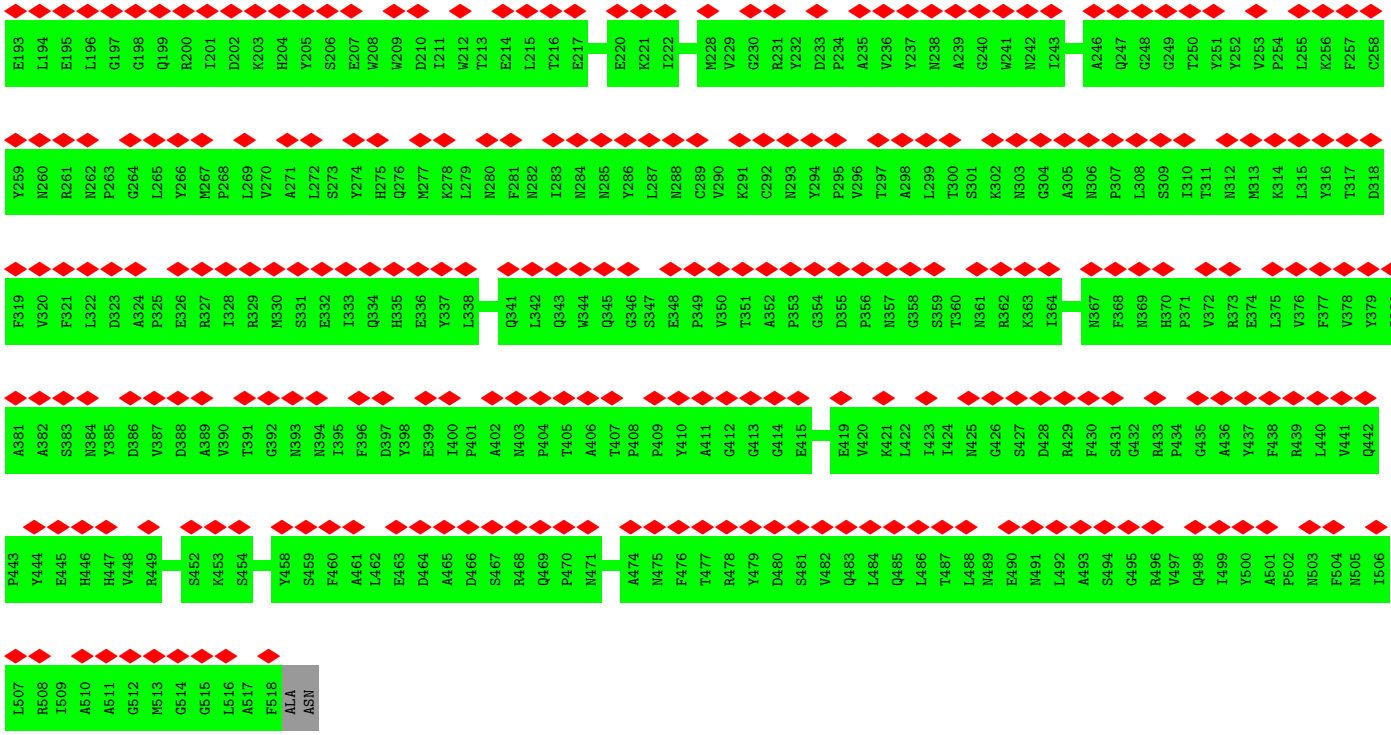
Chain bB:





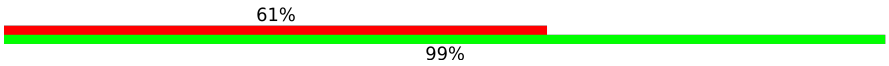


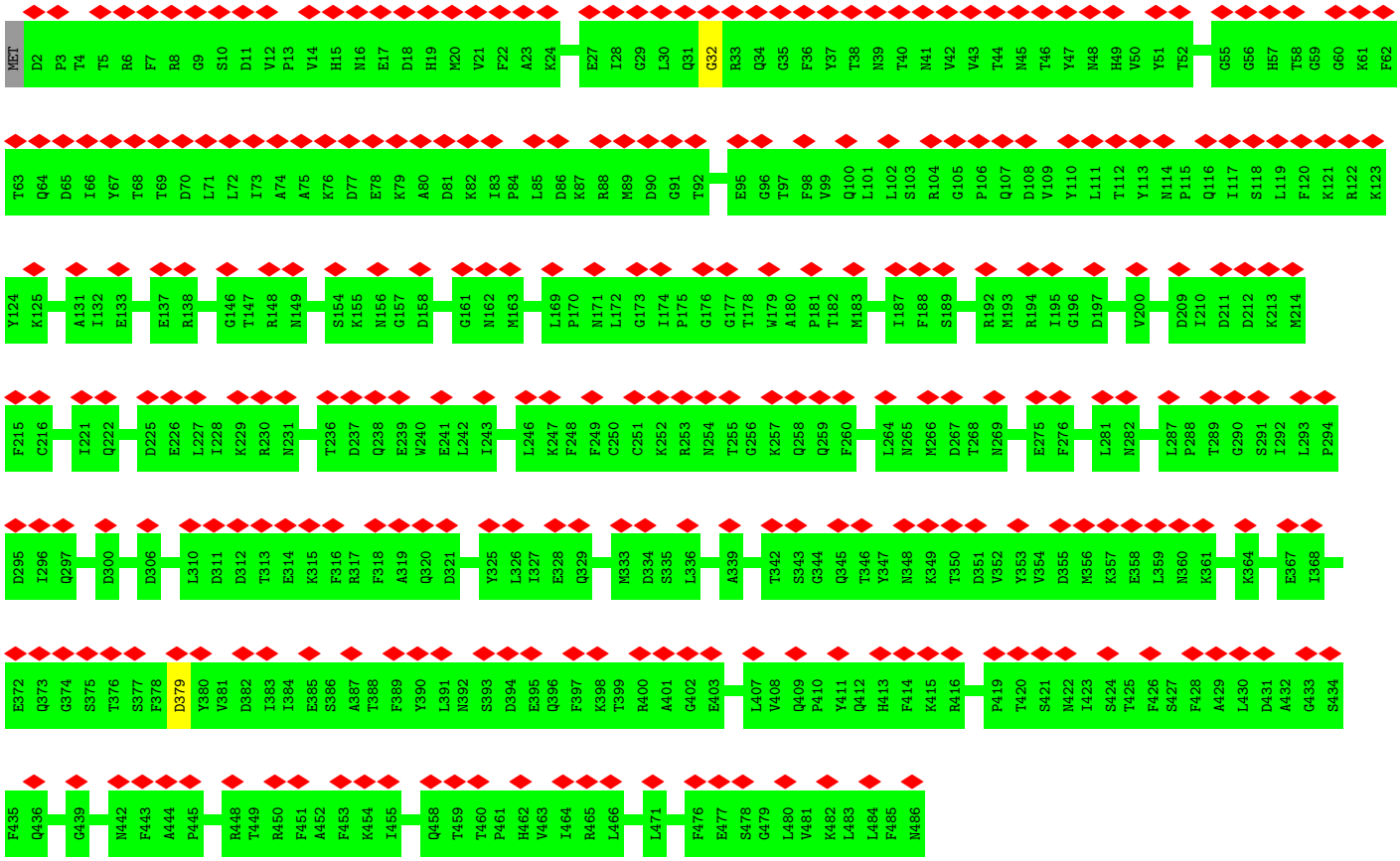




- Molecule 3: MCPv2

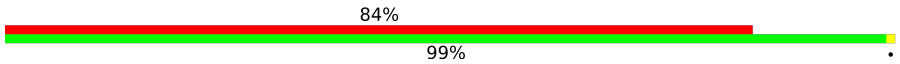
Chain bC:

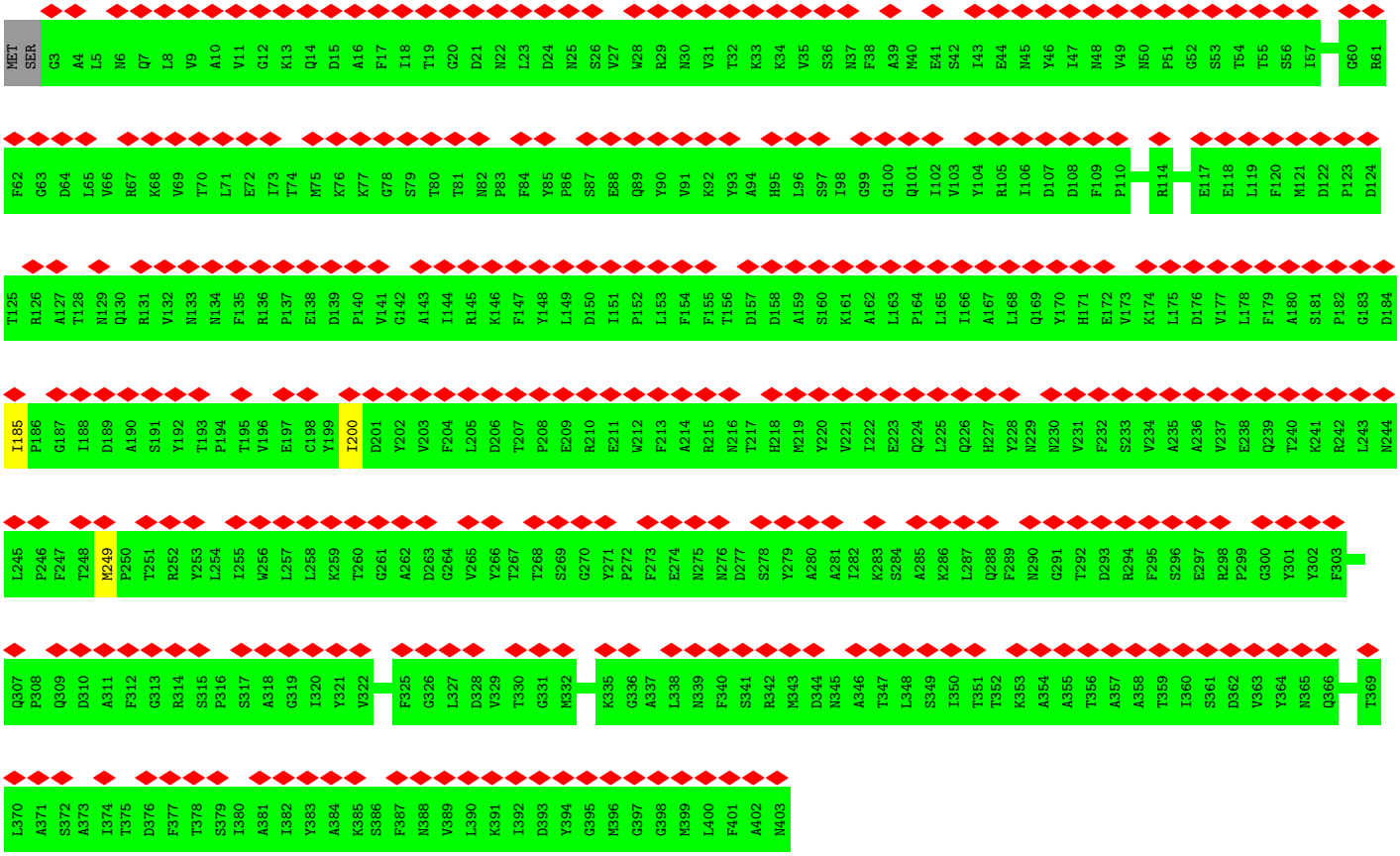




• Molecule 4: MCPv3

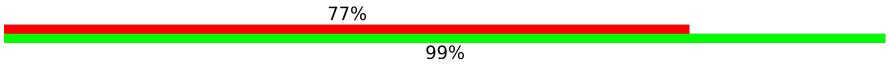
Chain bD:

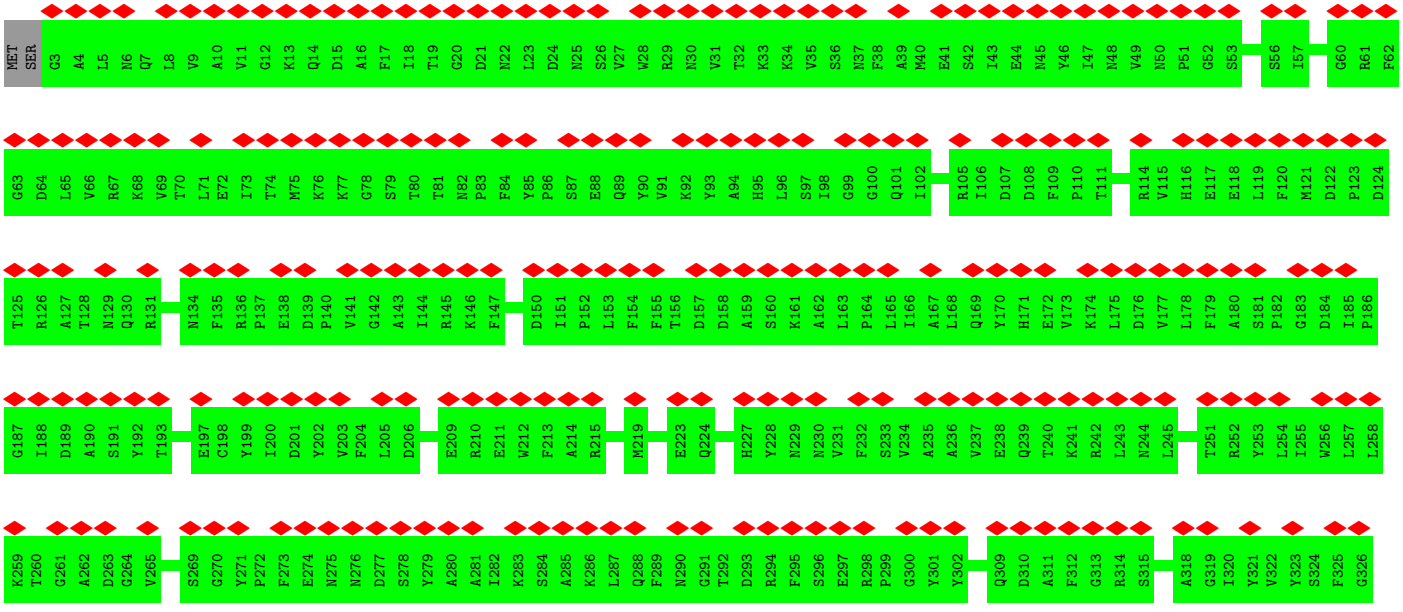


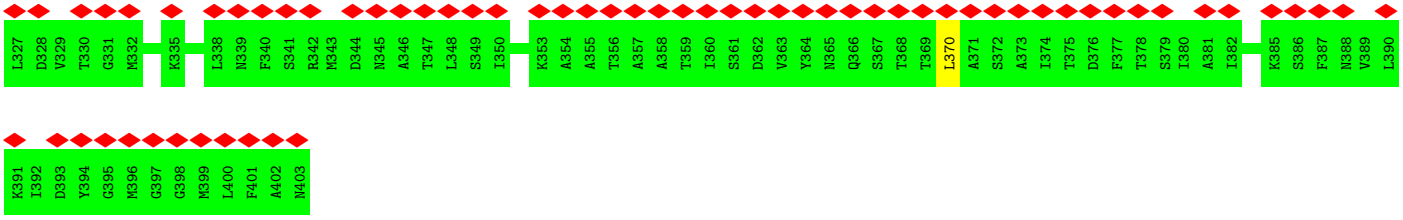


• Molecule 4: MCPv3

Chain bF:

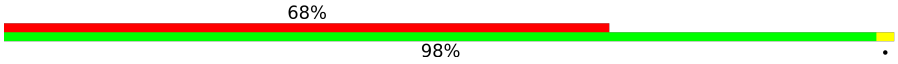


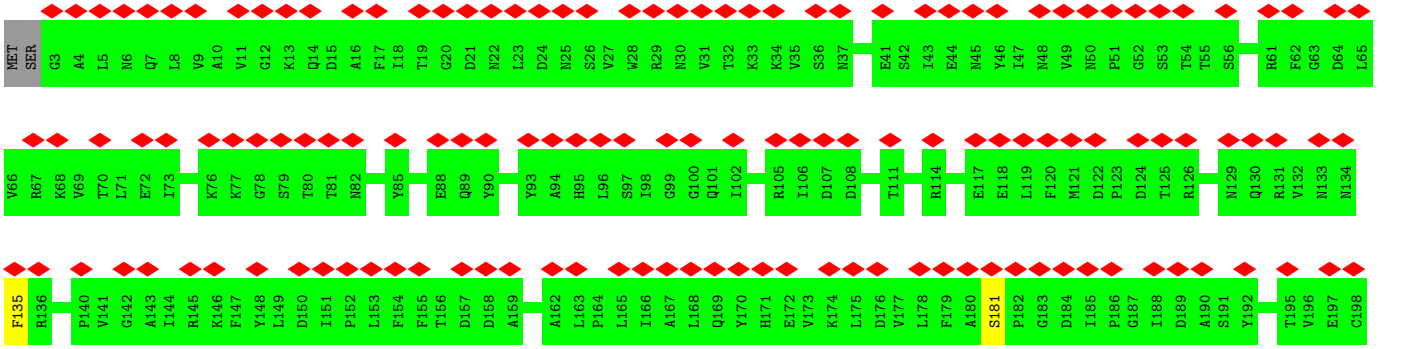




• Molecule 4: MCPv3

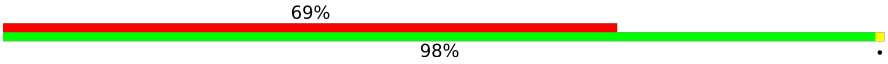
Chain cX:

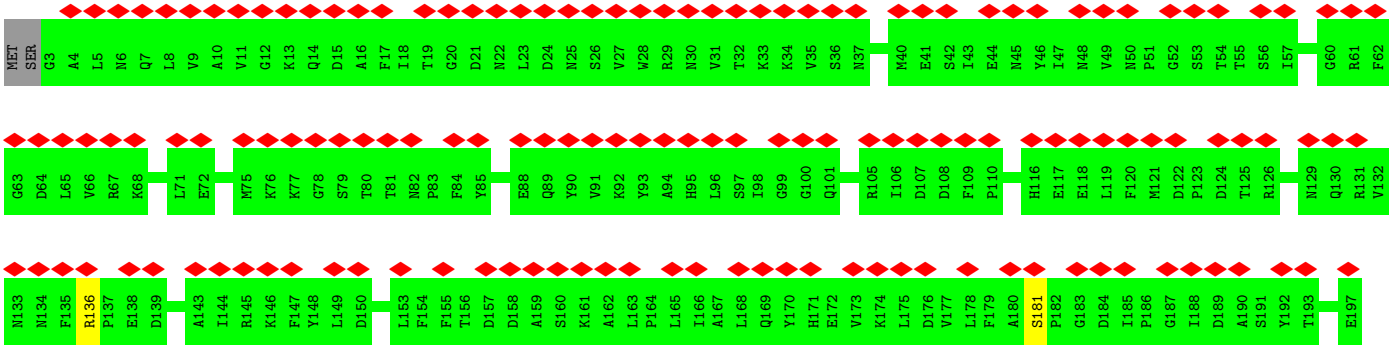


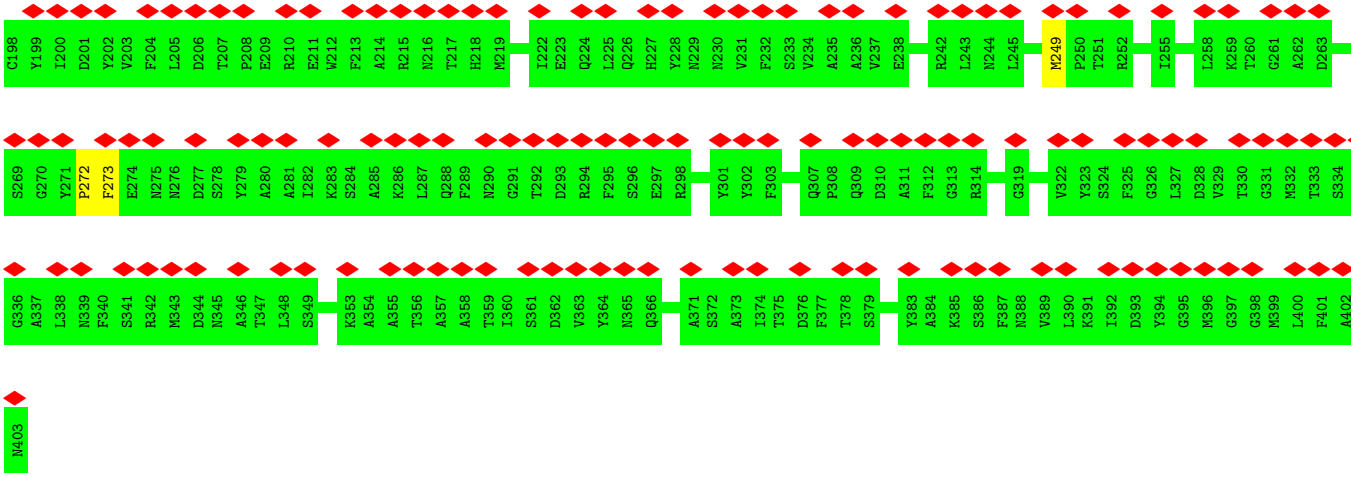


• Molecule 4: MCPv3

Chain cZ:

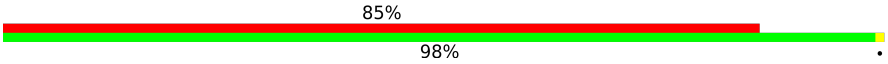


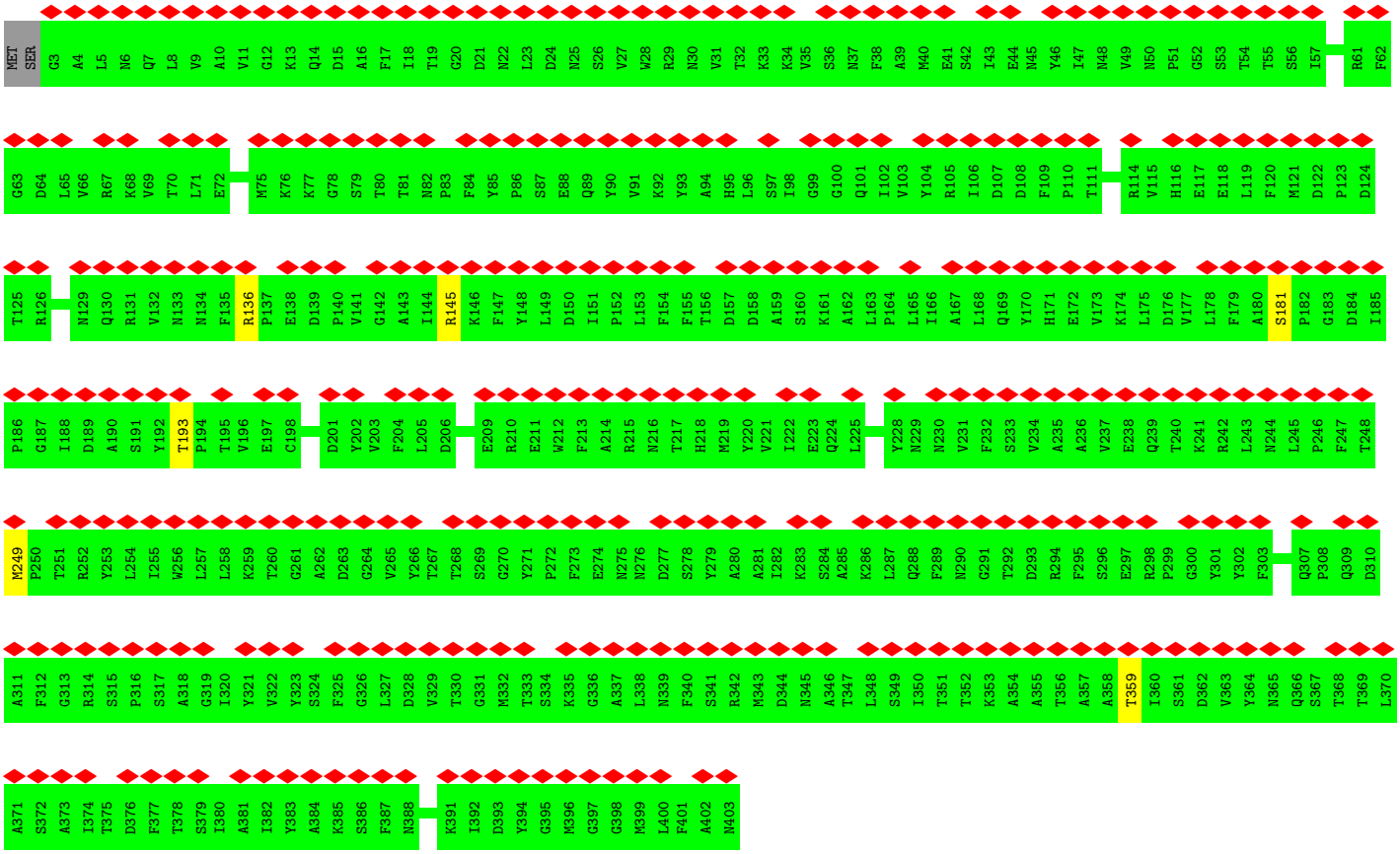




- Molecule 4: MCPv3

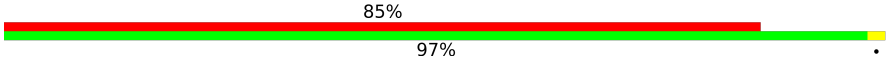
Chain dd:

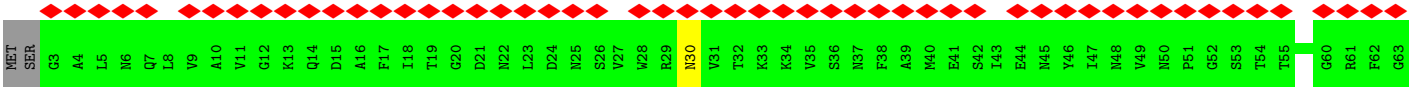


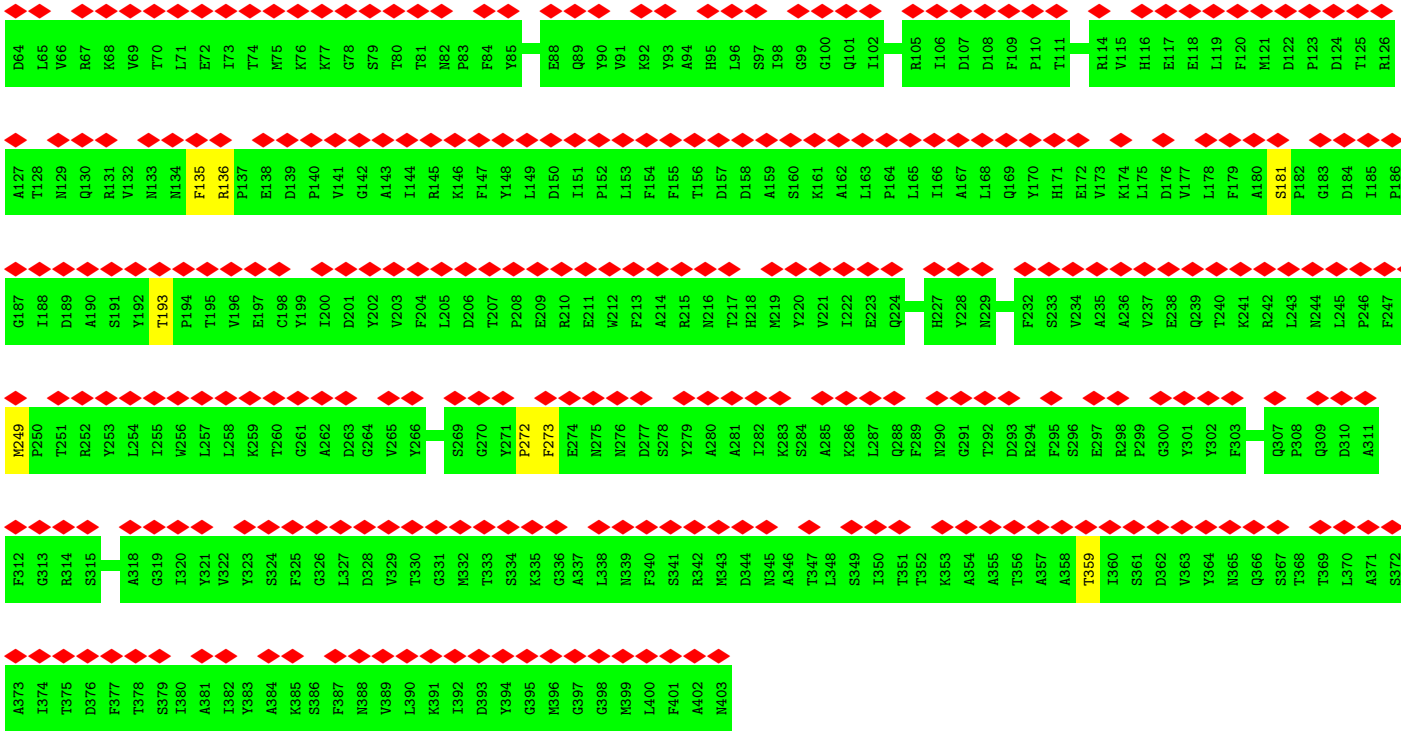


- Molecule 4: MCPv3

Chain df:

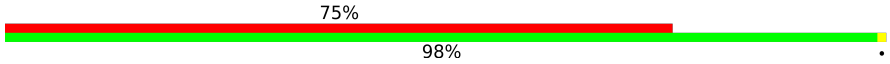


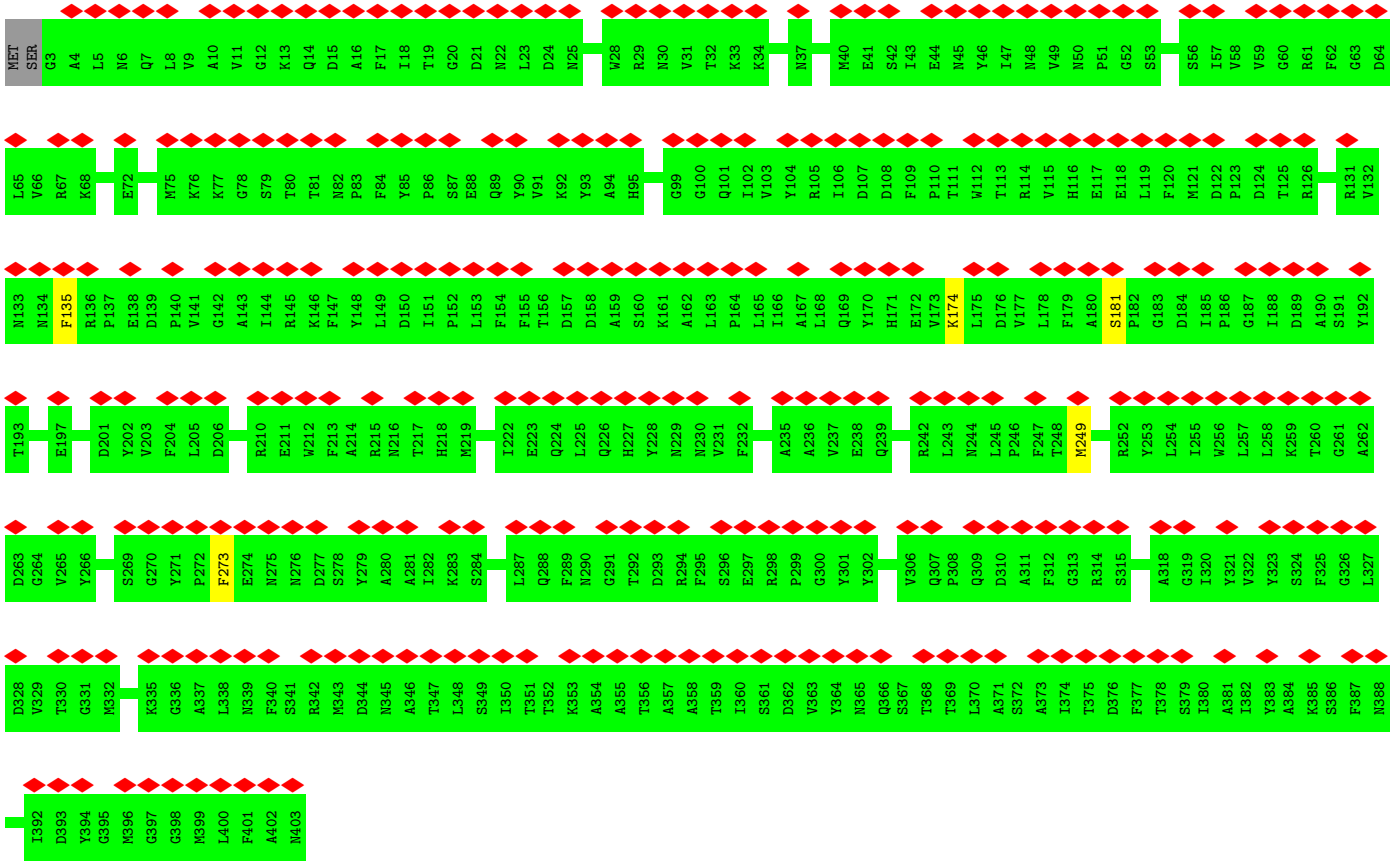




- Molecule 4: MCPv3

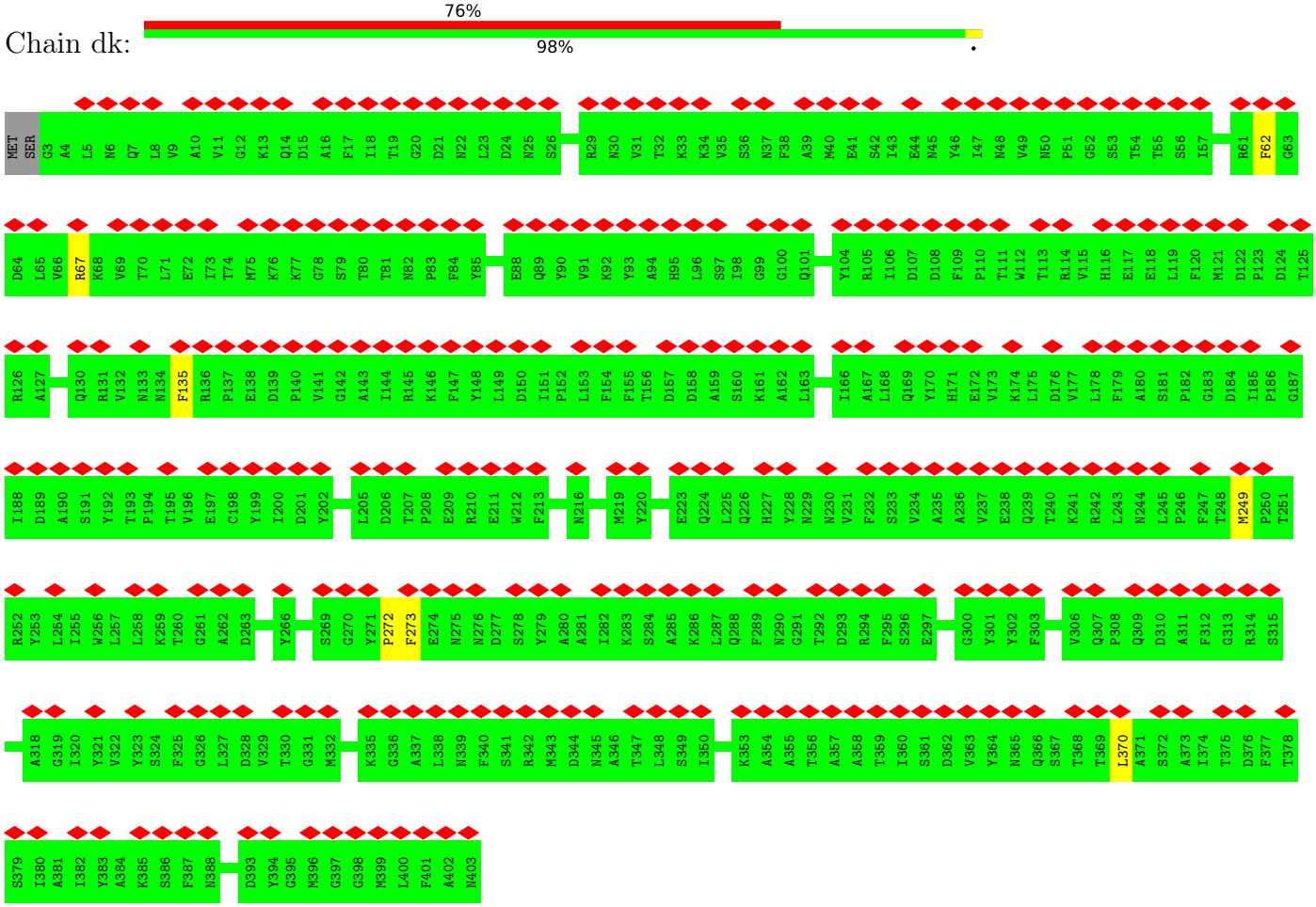
Chain dj:





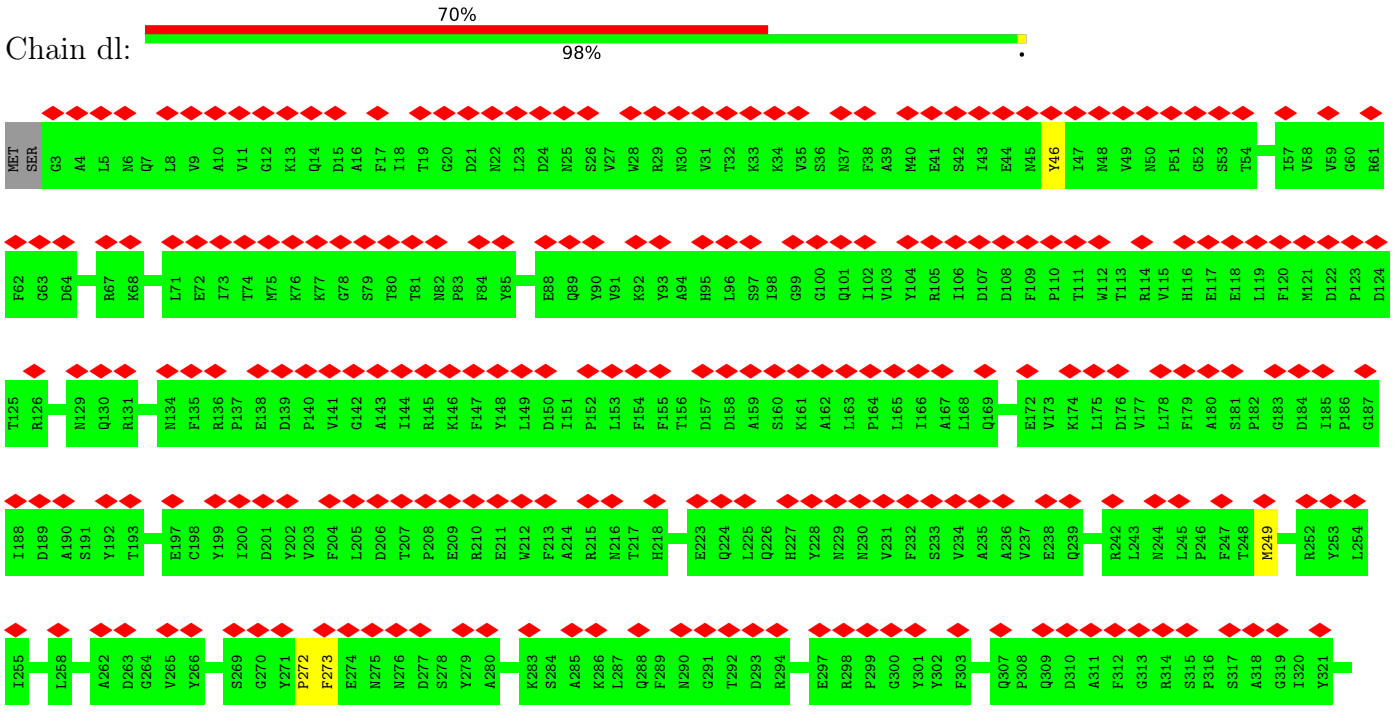
• Molecule 4: MCPv3

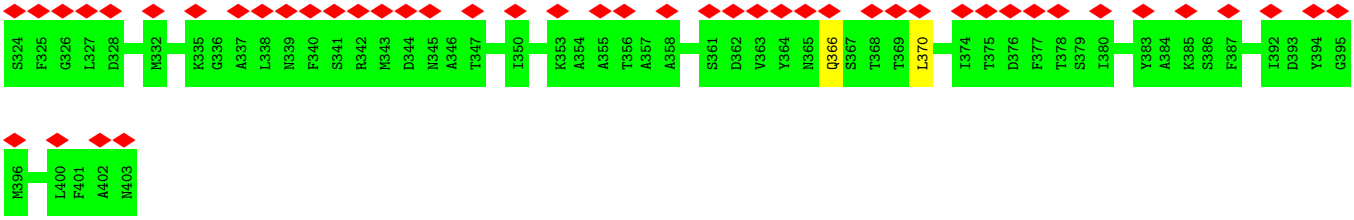
Chain dk:



• Molecule 4: MCPv3

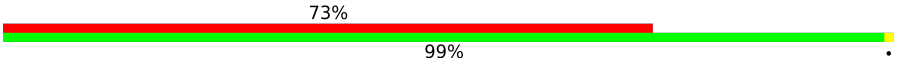
Chain dl:

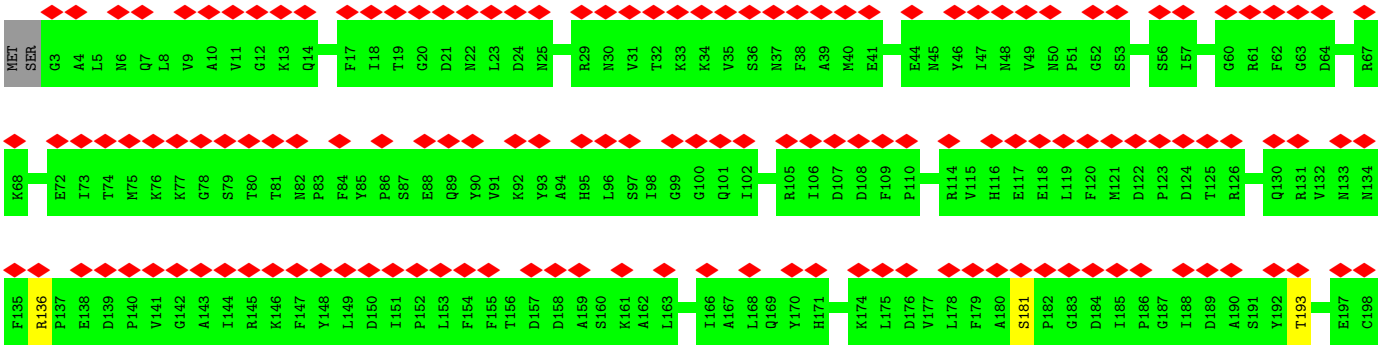




• Molecule 4: MCPv3

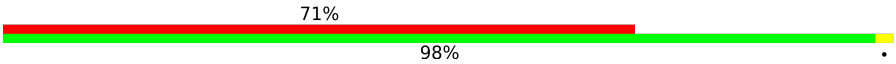
Chain dp:

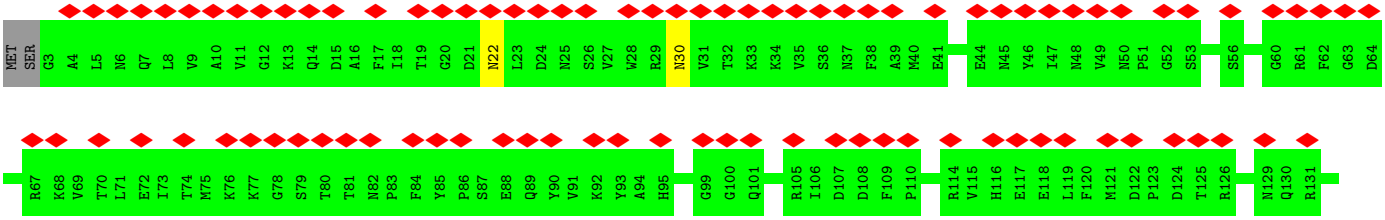




• Molecule 4: MCPv3

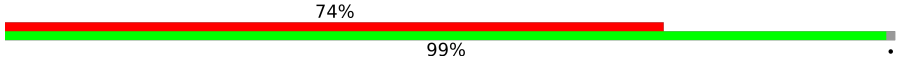
Chain dr:

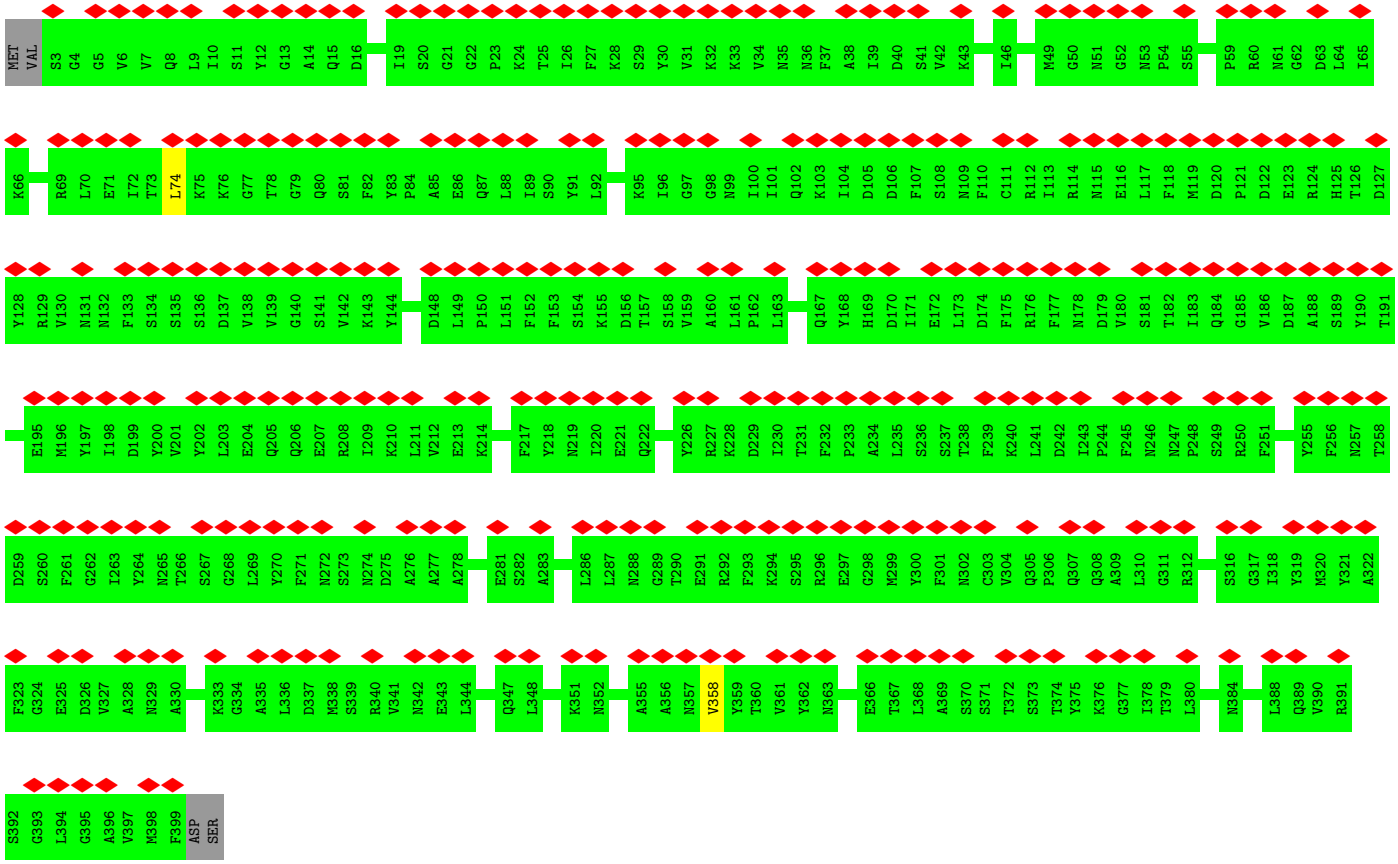




• Molecule 5: MCPv4

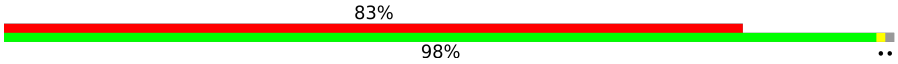
Chain bE:

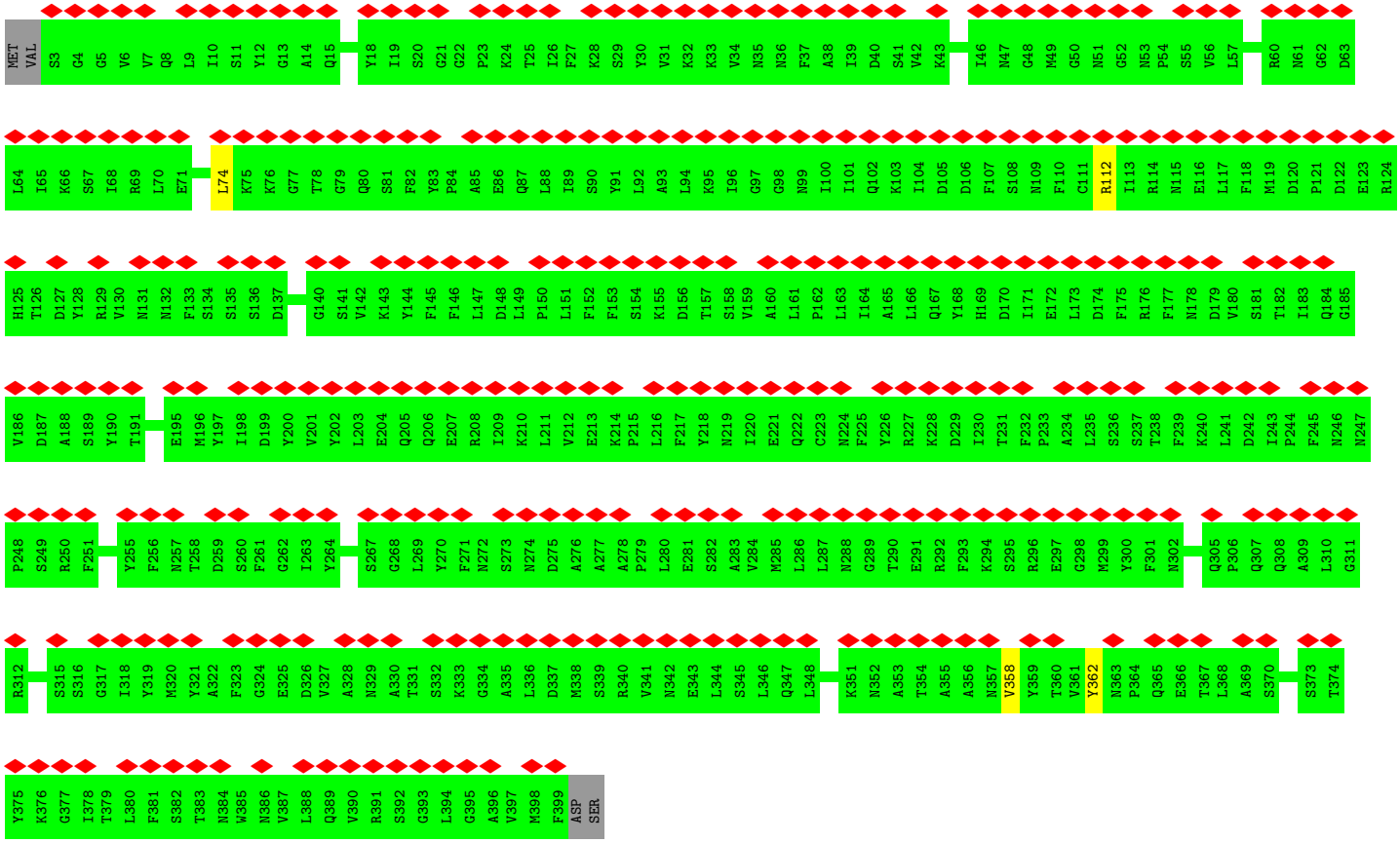




• Molecule 5: MCPv4

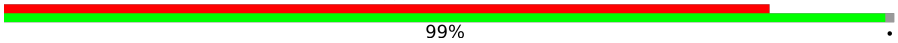
Chain cY:

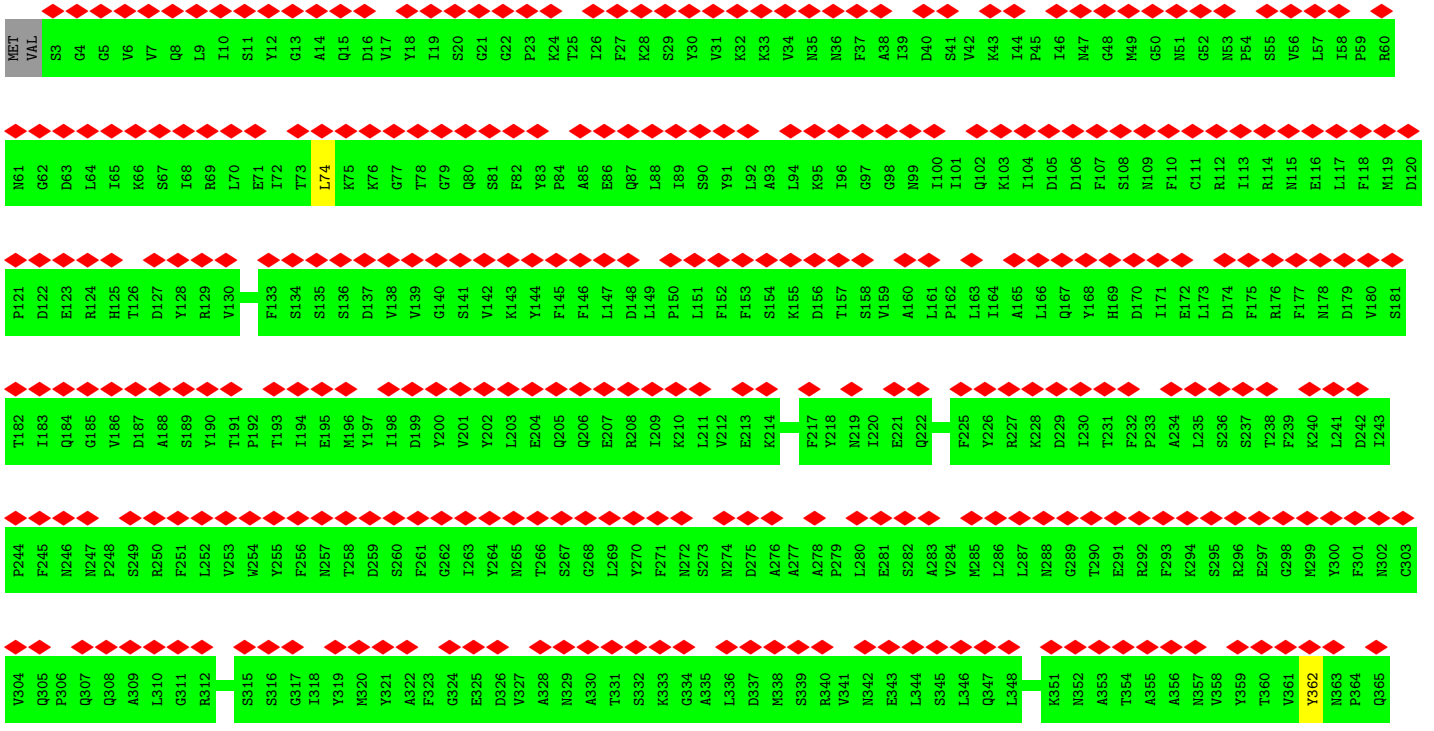


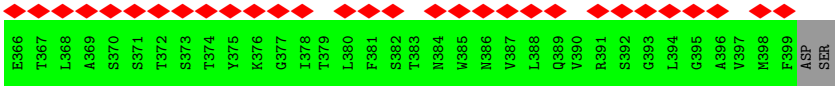


• Molecule 5: MCPv4

Chain de:

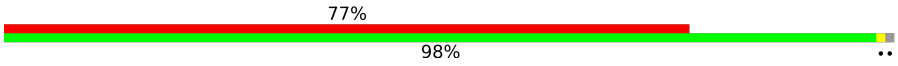


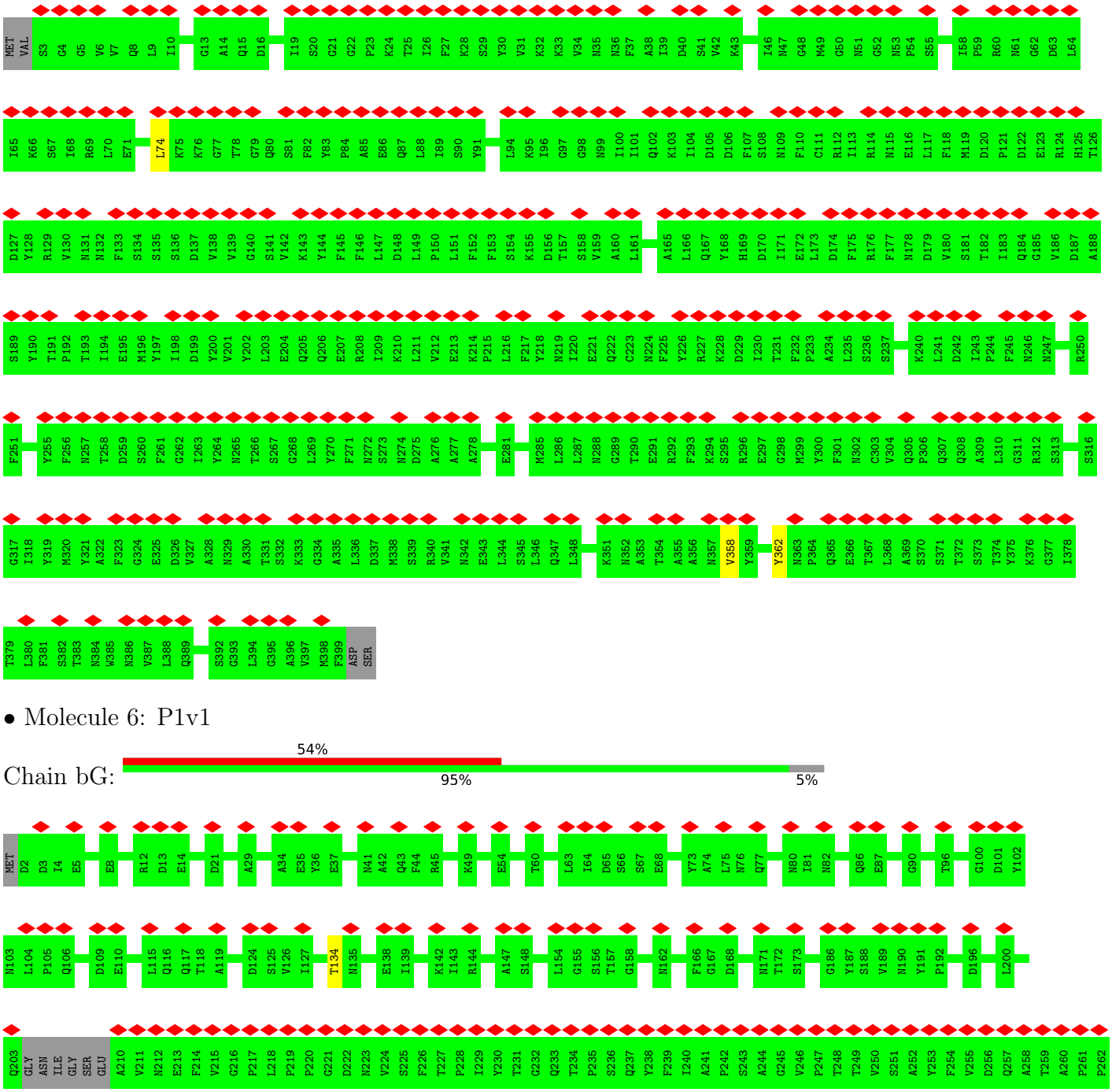




• Molecule 5: MCPv4

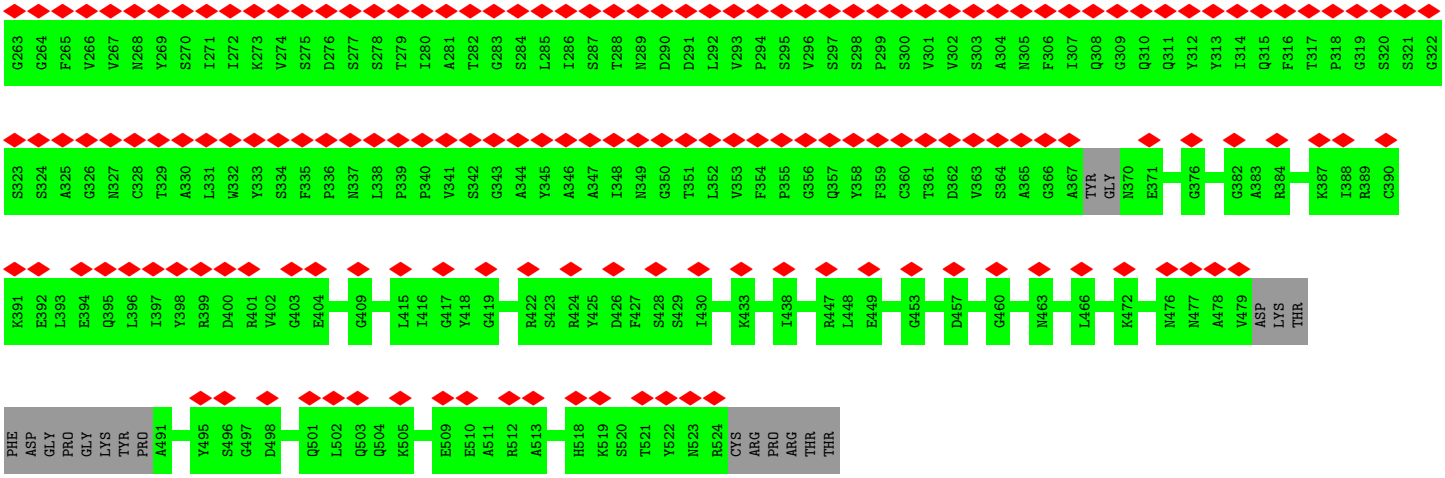
Chain dq:





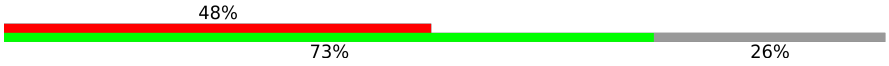
• Molecule 6: P1v1

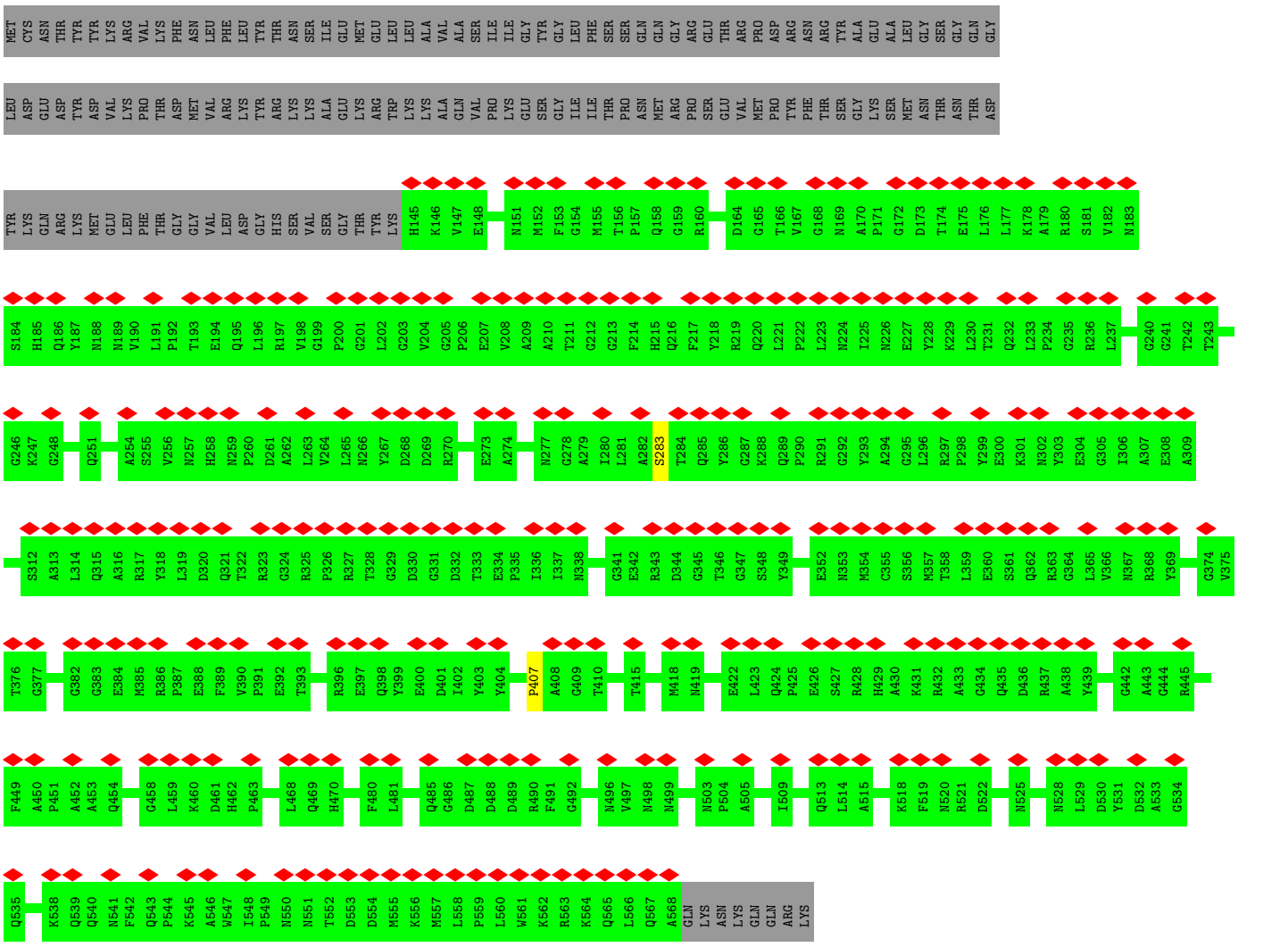
Chain bG:



• Molecule 7: P2

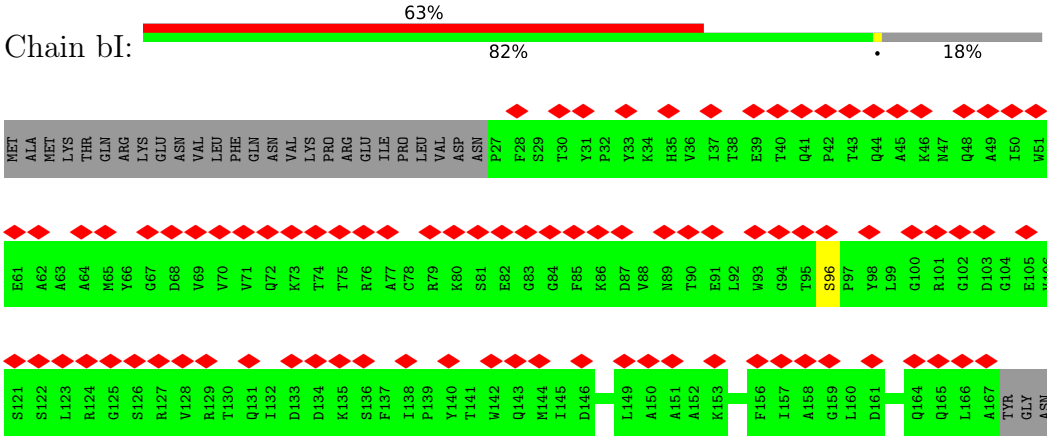
Chain bH:





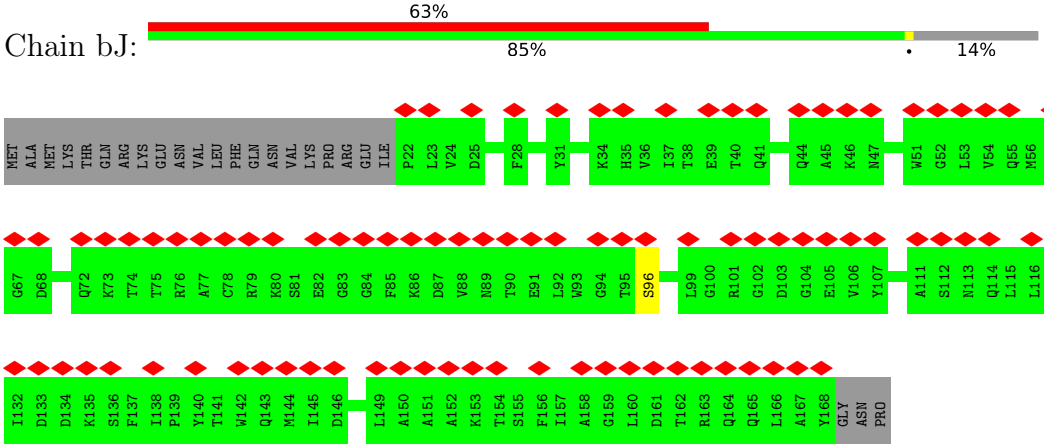
• Molecule 8: P3

Chain bI:



• Molecule 8: P3

Chain bJ:



• Molecule 8: P3

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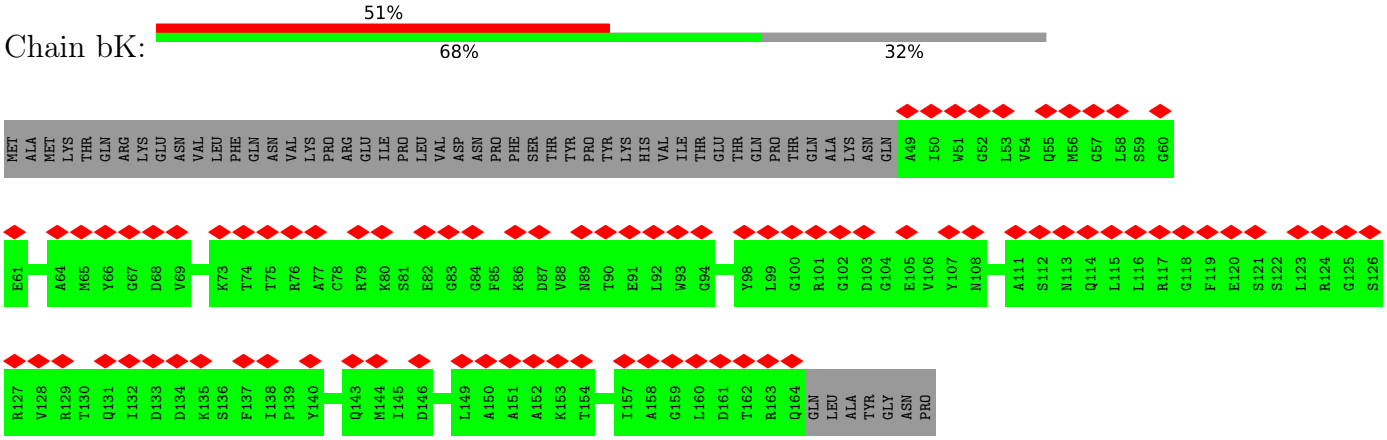
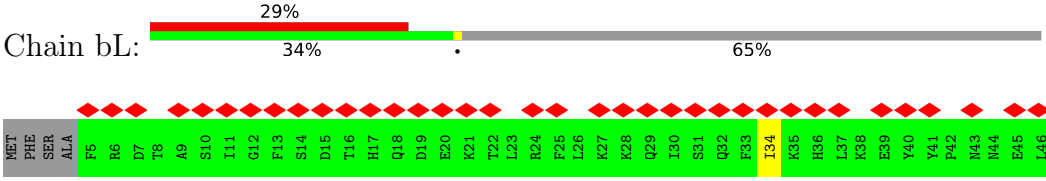
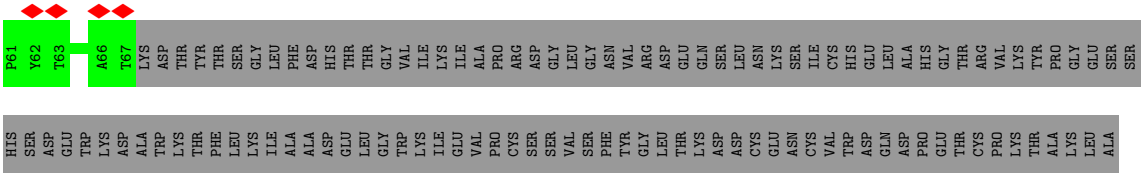


• Molecule 9: P4

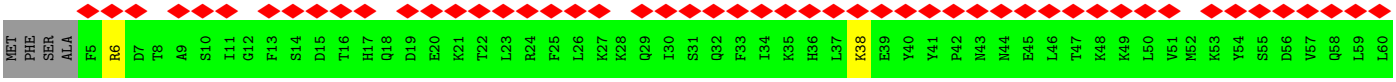
Chain bL:

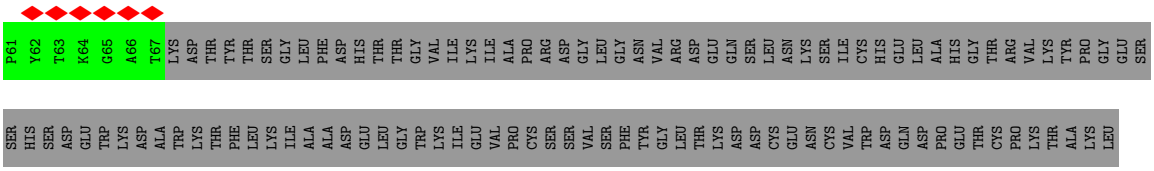




• Molecule 9: P4

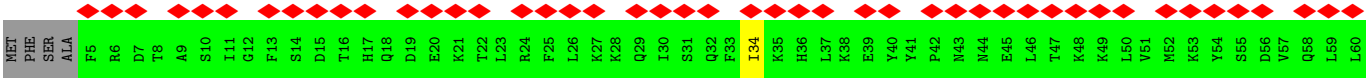
Chain bM:

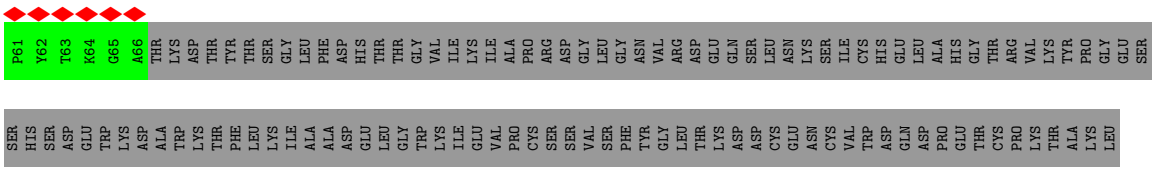




• Molecule 9: P4

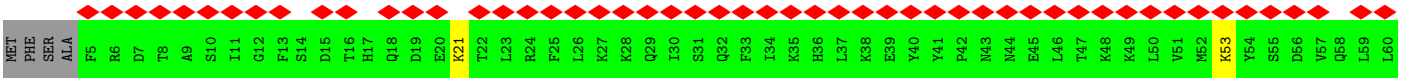
Chain bN:

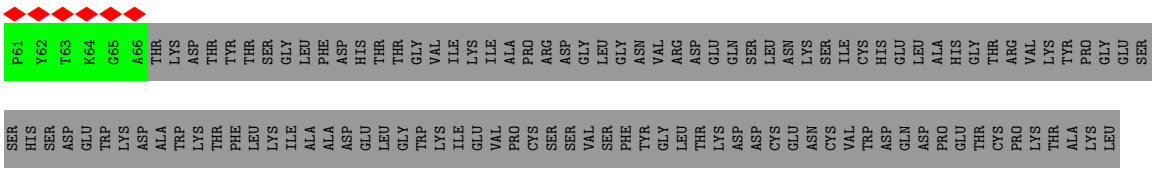




• Molecule 9: P4

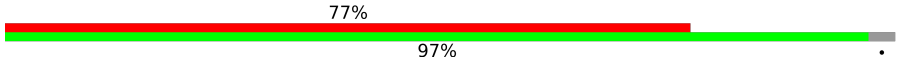
Chain bO:

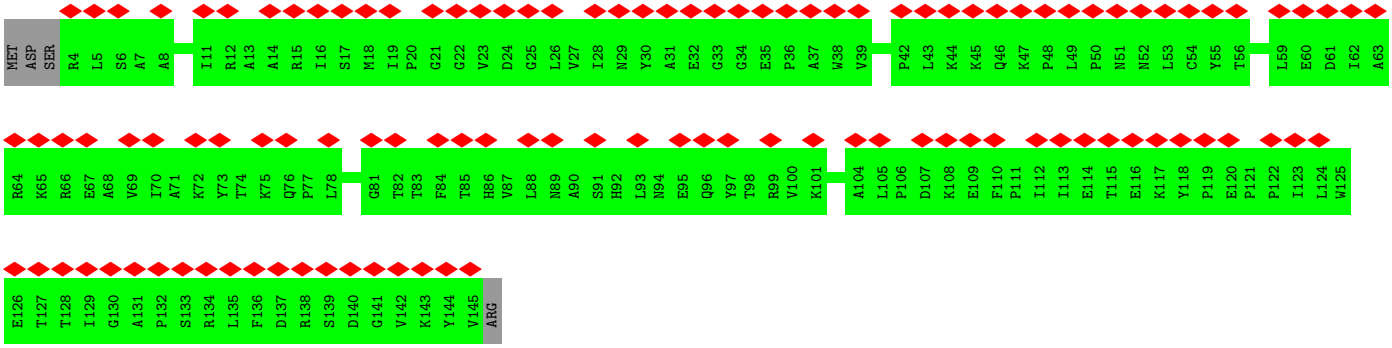




• Molecule 10: P5

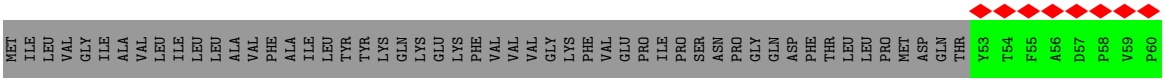
Chain bP:

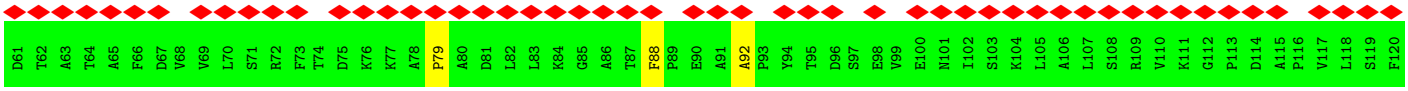


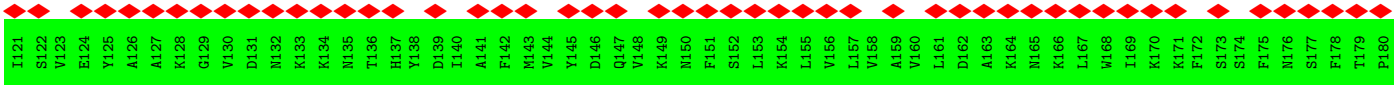


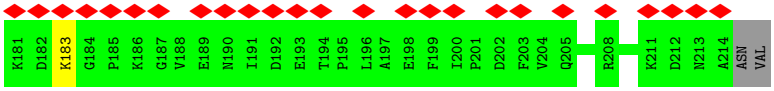
• Molecule 11: P6

Chain bQ:



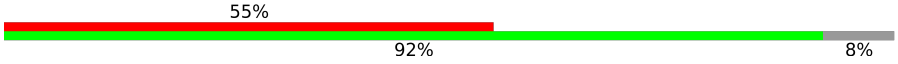


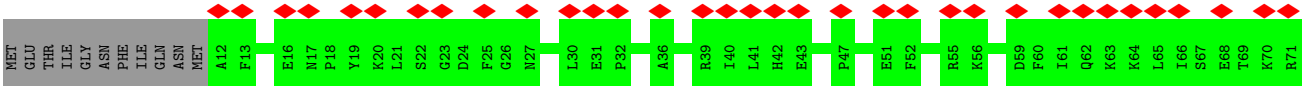


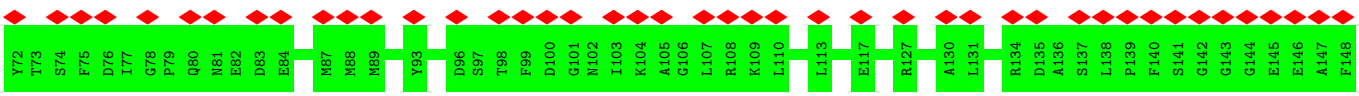


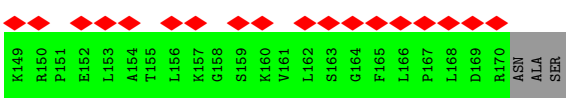
• Molecule 12: P8

Chain bR:



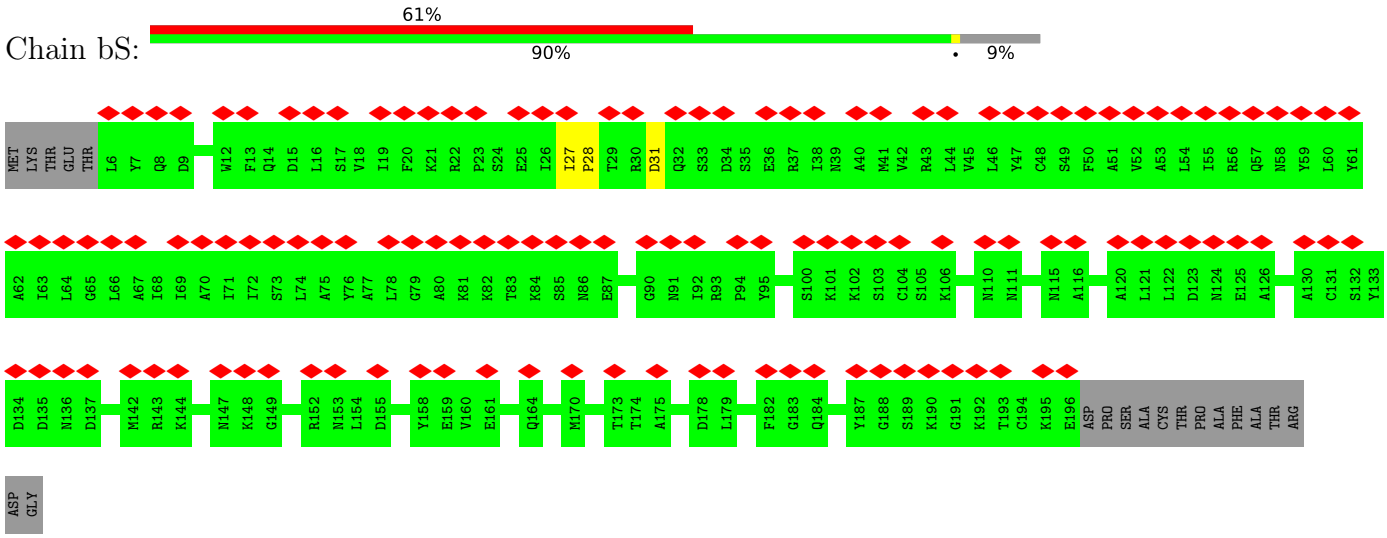






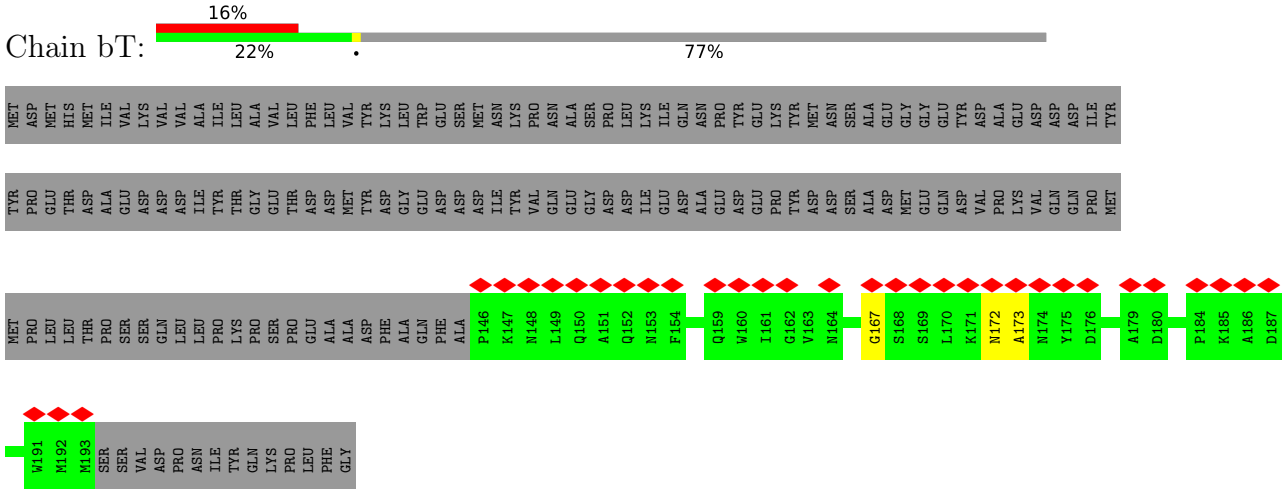
• Molecule 13: P9

Chain bS:



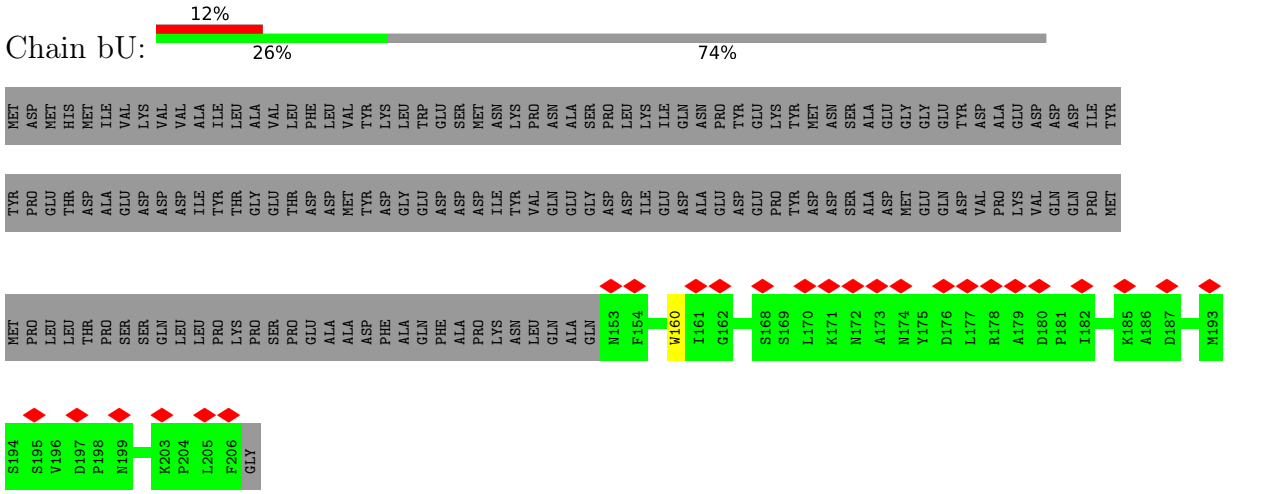
• Molecule 14: P11

Chain bT:



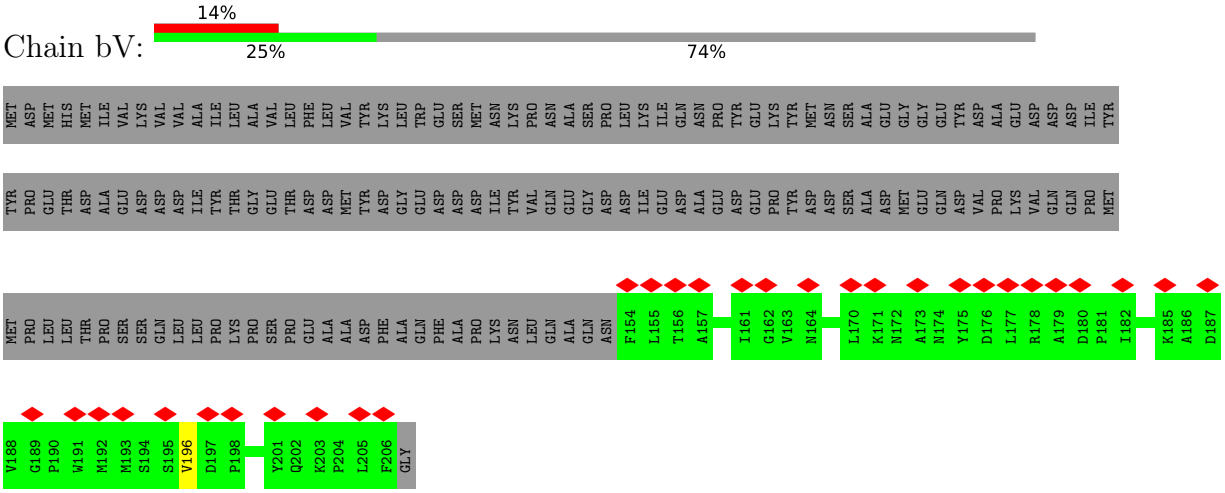
• Molecule 14: P11

Chain bU:



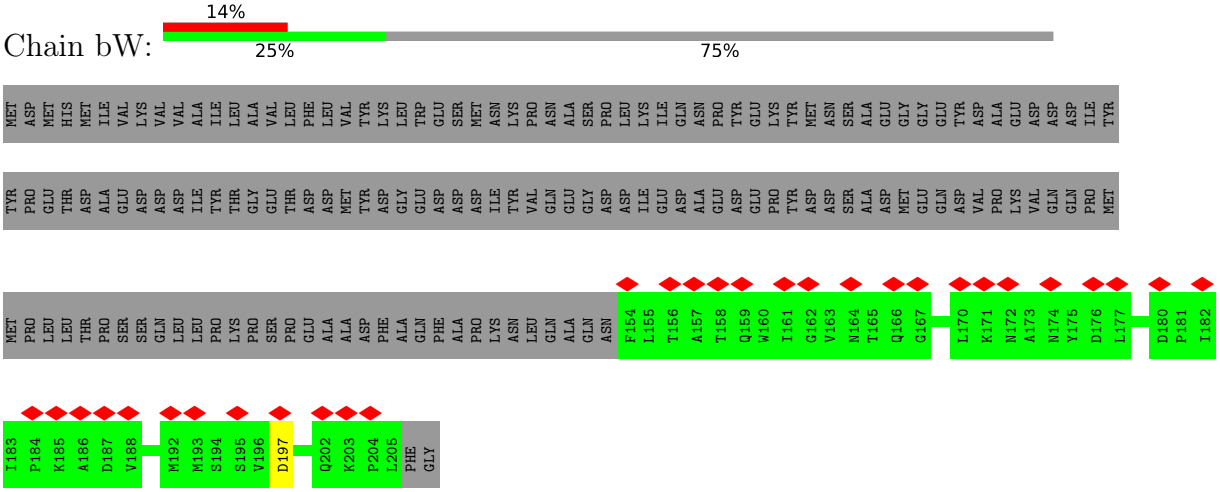
• Molecule 14: P11

Chain bV:



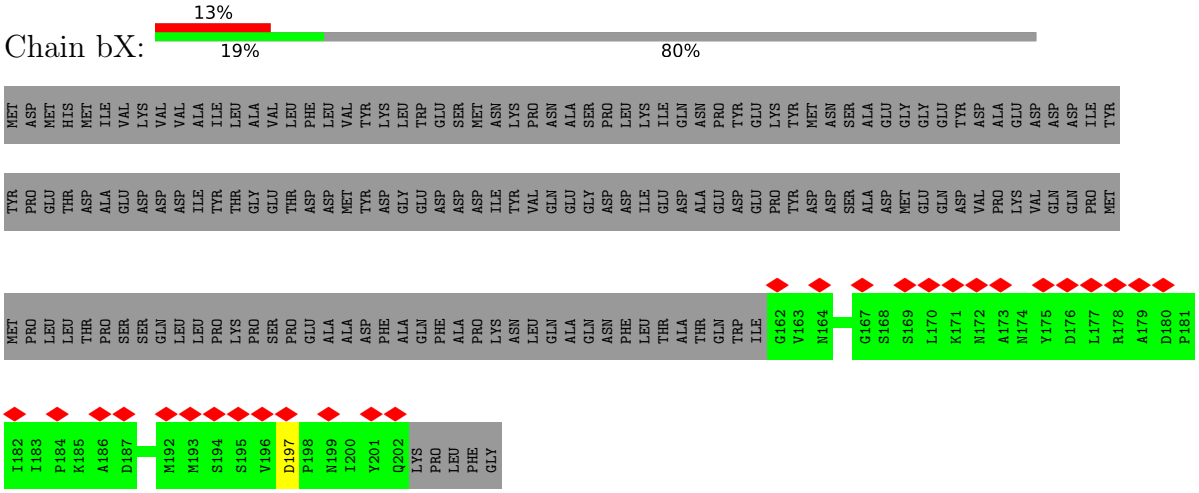
• Molecule 14: P11

Chain bW:



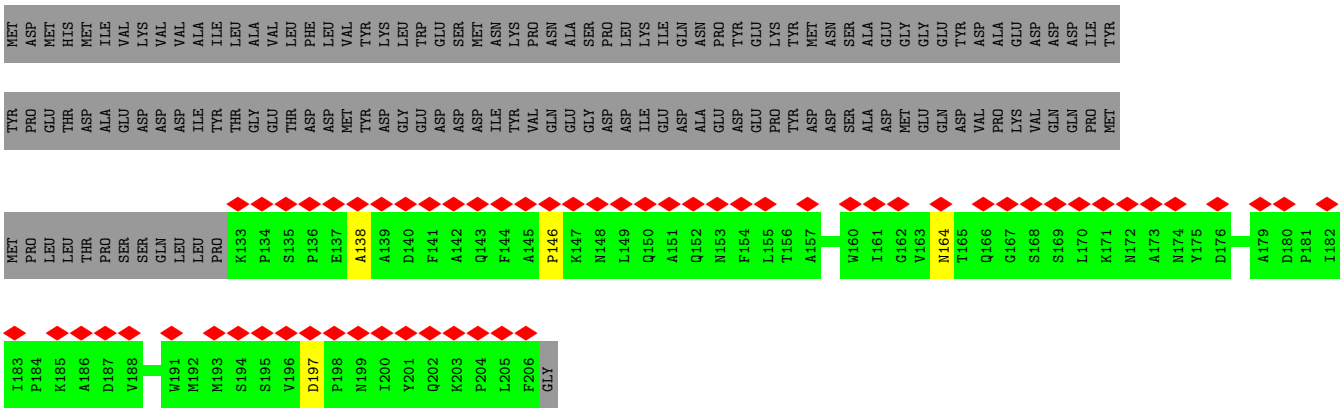
• Molecule 14: P11

Chain bX:



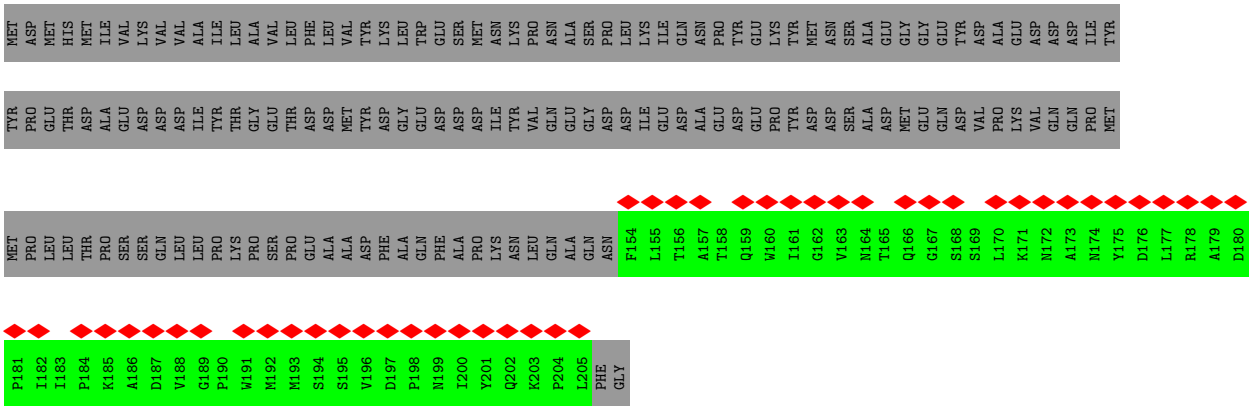
• Molecule 14: P11

Chain bY:



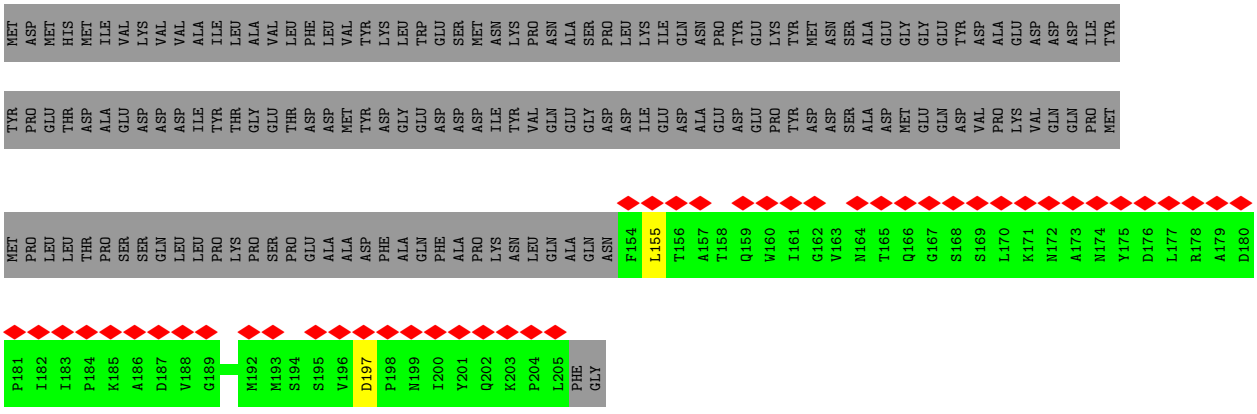
- Molecule 14: P11

Chain bZ:



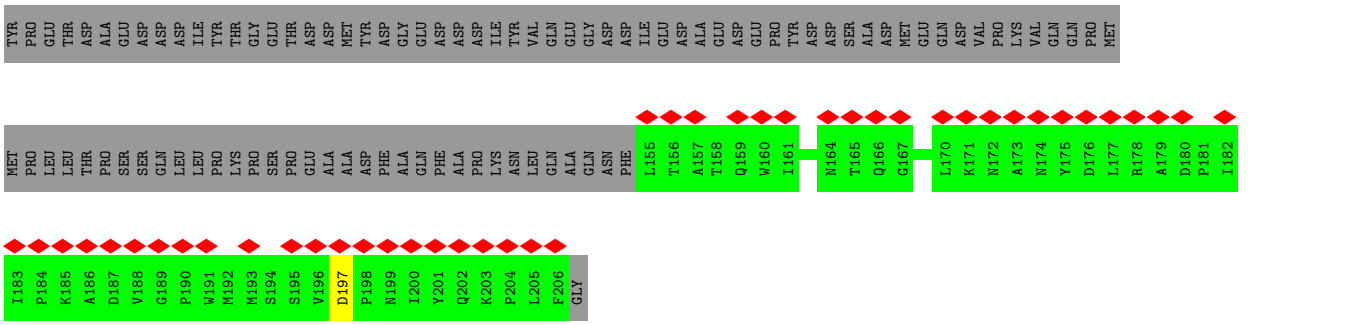
- Molecule 14: P11

Chain ca:

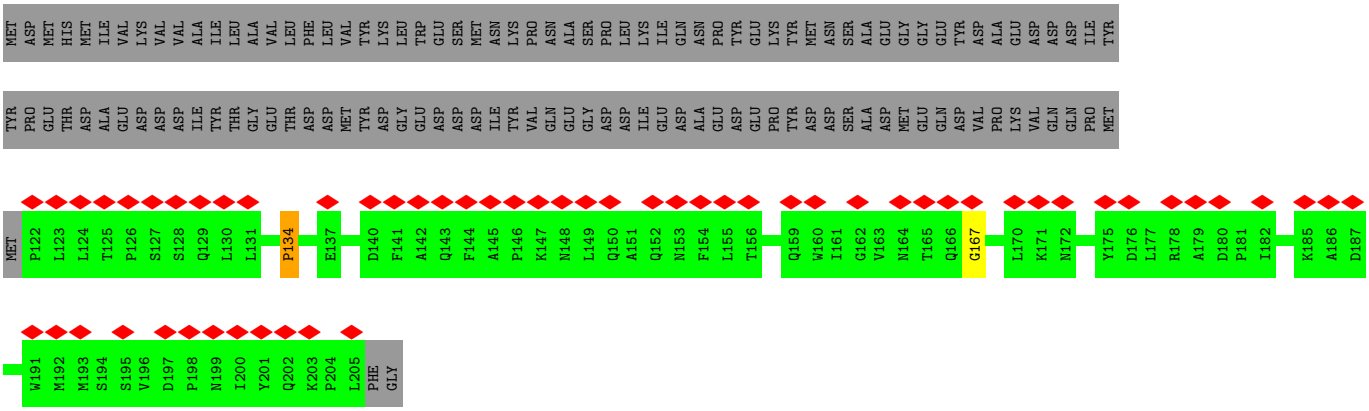


- Molecule 14: P11

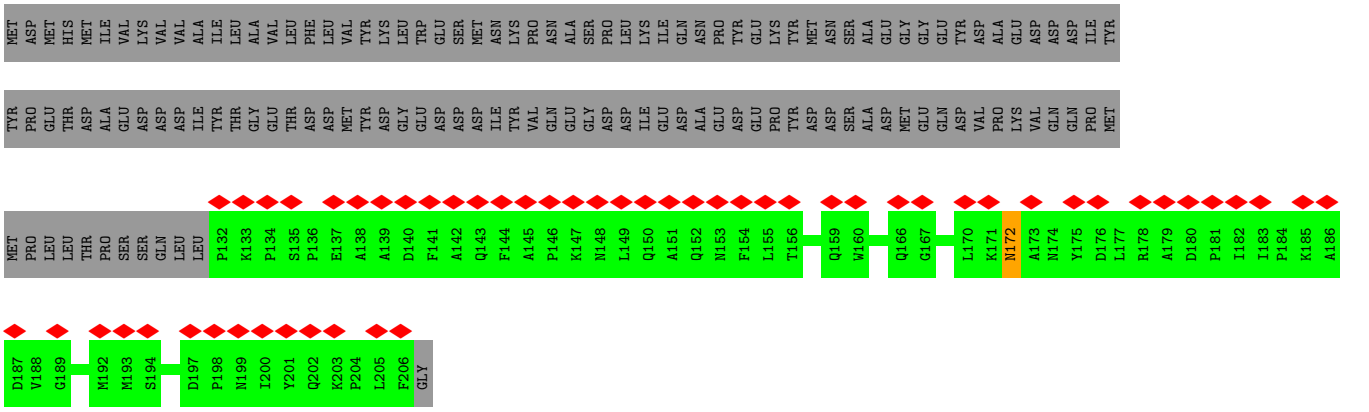
Chain cb:



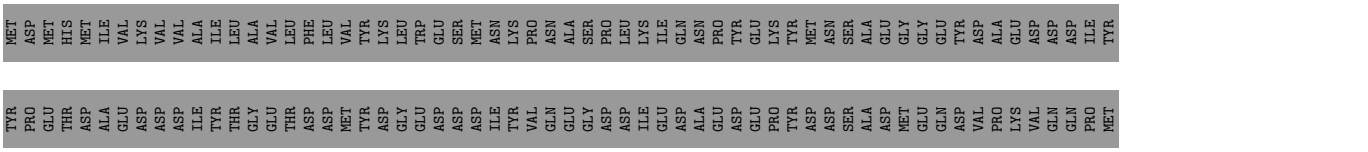
• Molecule 14: P11

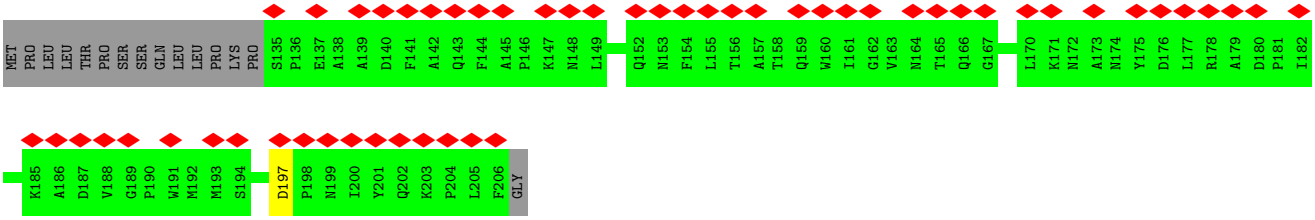


• Molecule 14: P11



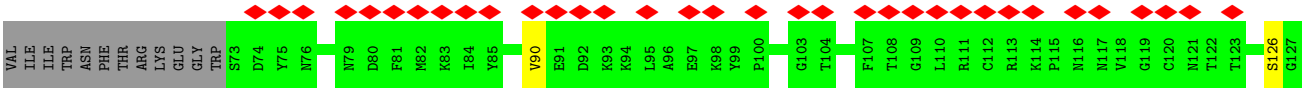
• Molecule 14: P11

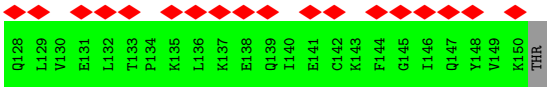




- Molecule 15: P12

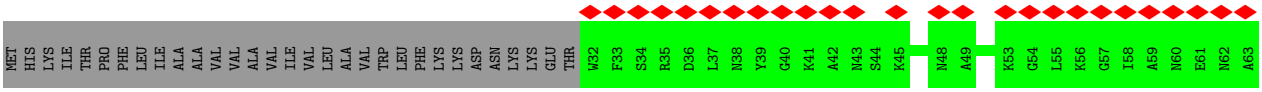
Chain cf:

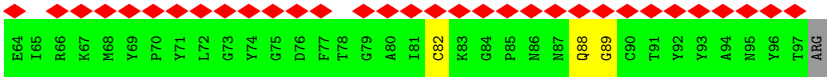




- Molecule 16: P13

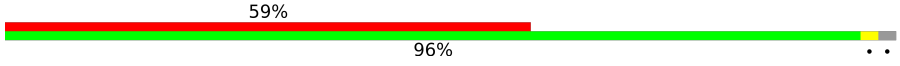
Chain cg:

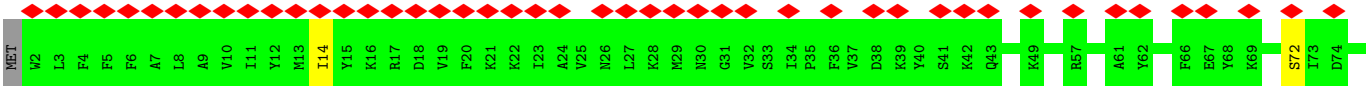


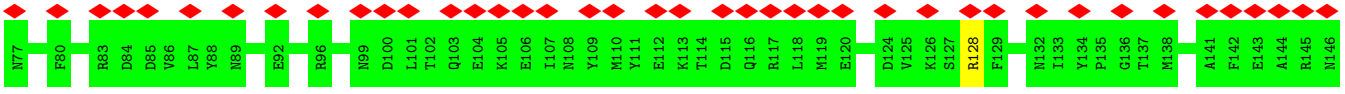


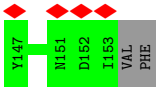
- Molecule 17: P15

Chain ch:



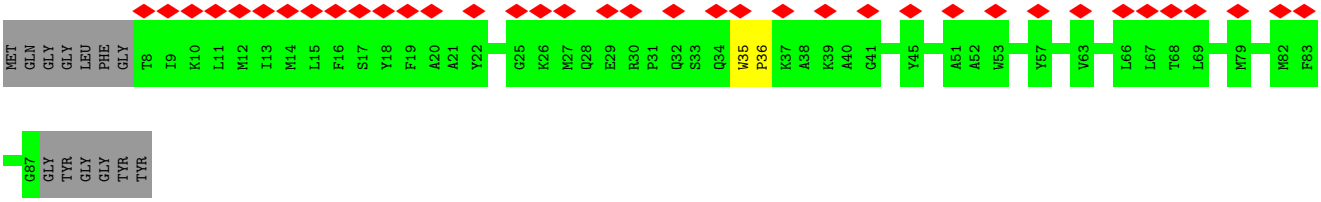






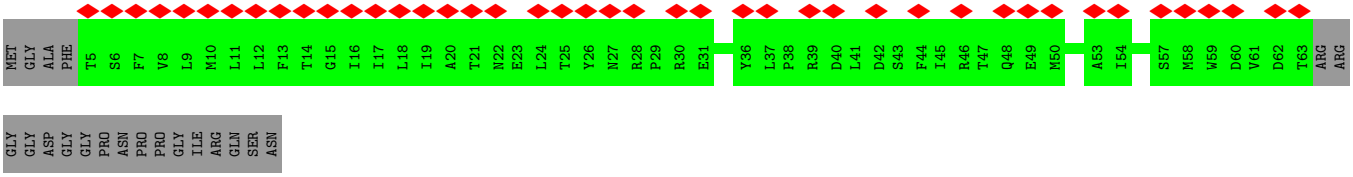
- Molecule 18: P16

Chain ci:



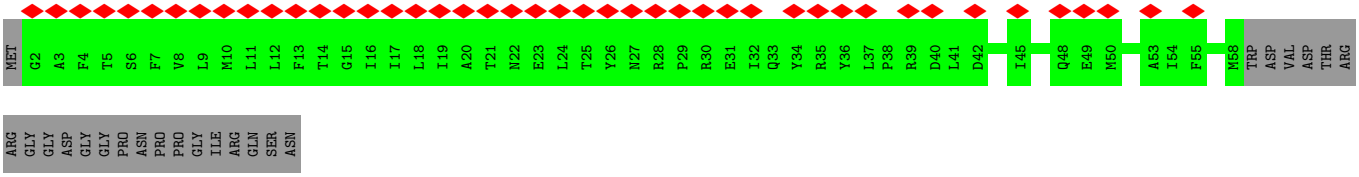
• Molecule 19: P17

Chain cj:



• Molecule 19: P17

Chain ck:



• Molecule 19: P17

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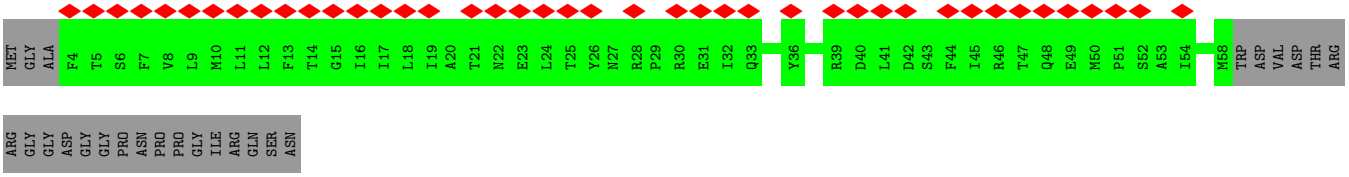
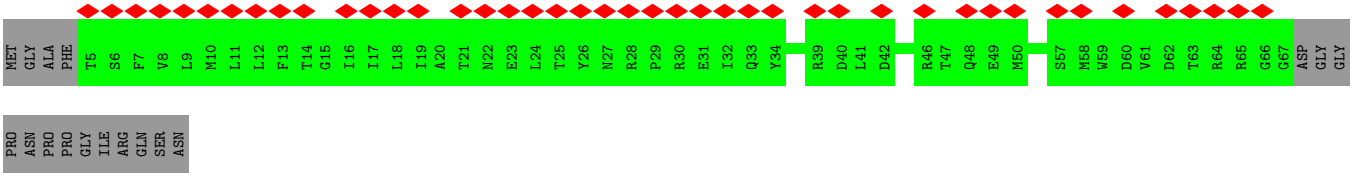


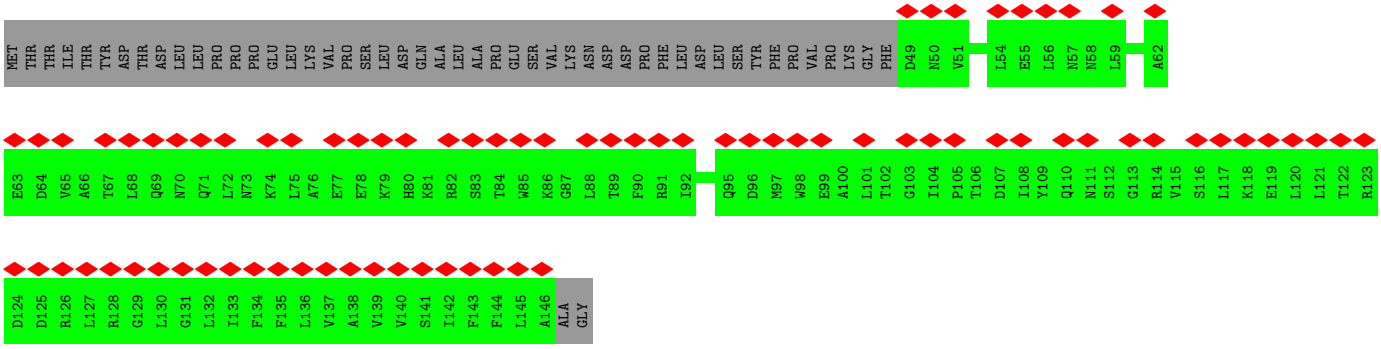
• Molecule 19: P17

Chain cm:



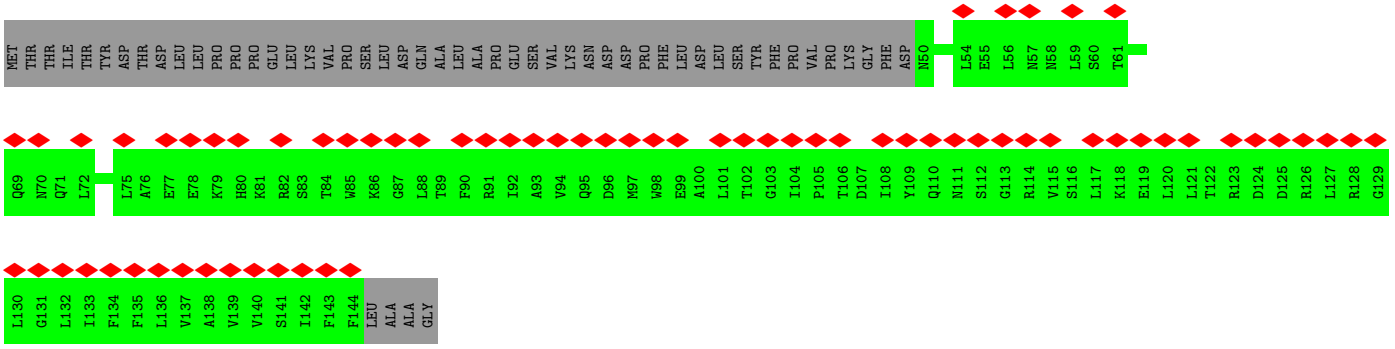
• Molecule 20: P18

Chain cn:



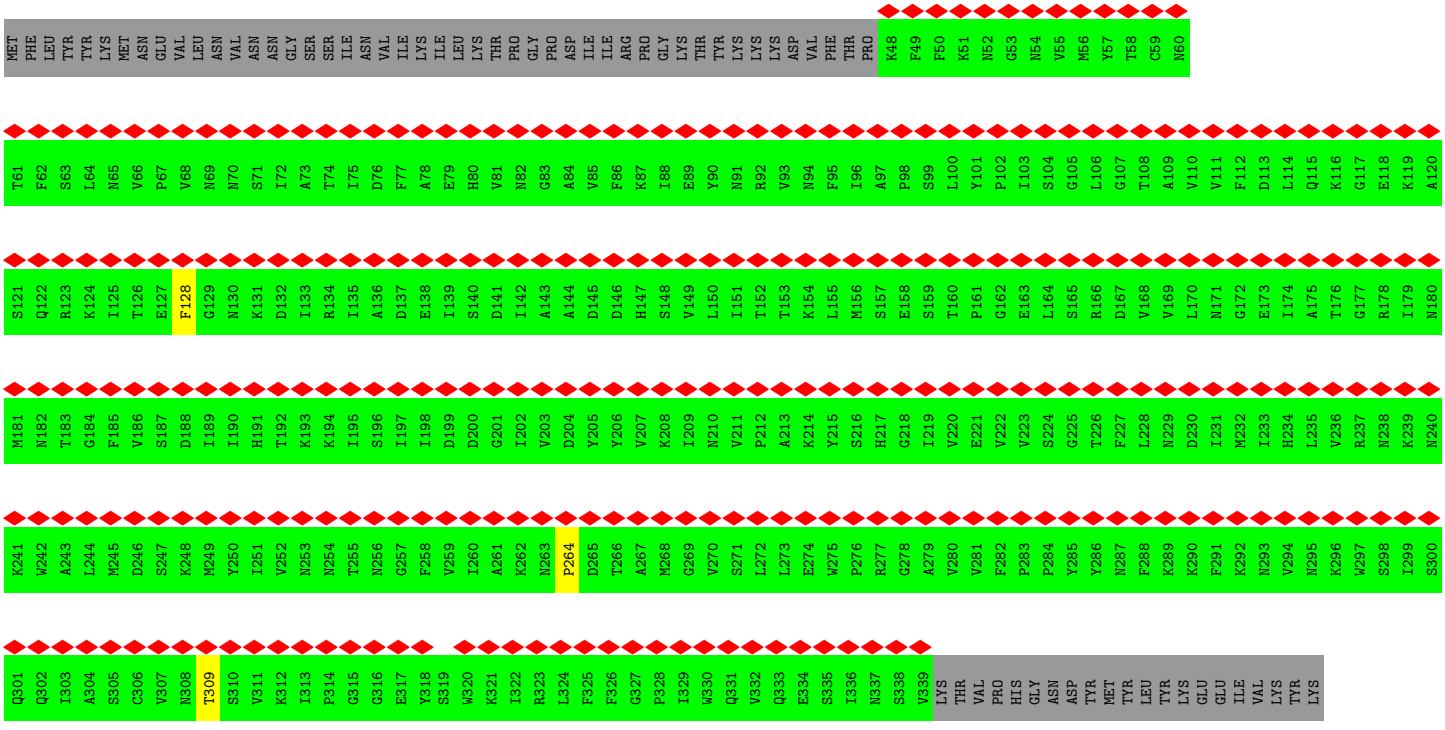
- Molecule 20: P18

Chain co:



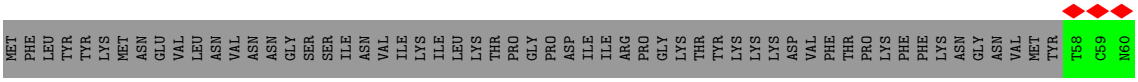
- Molecule 21: P19

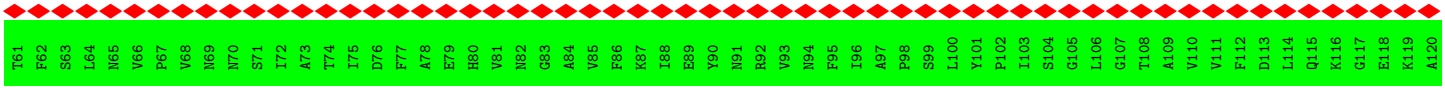
Chain cp:

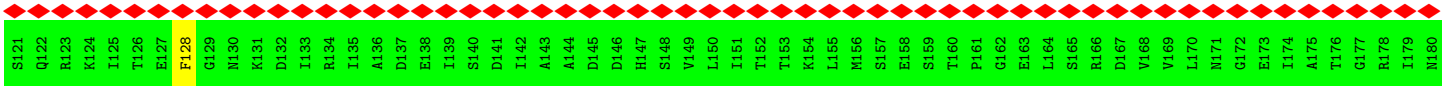


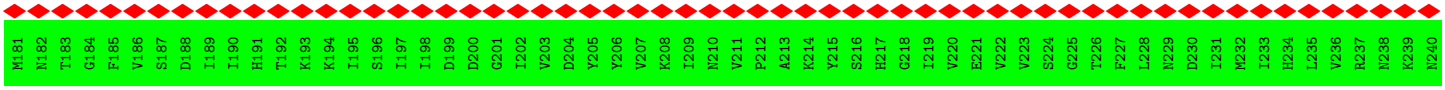
• Molecule 21: P19

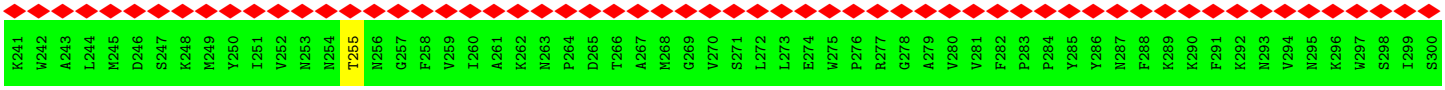
Chain cq:

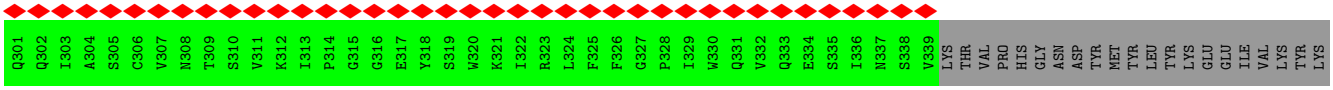






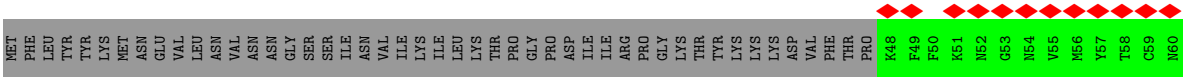


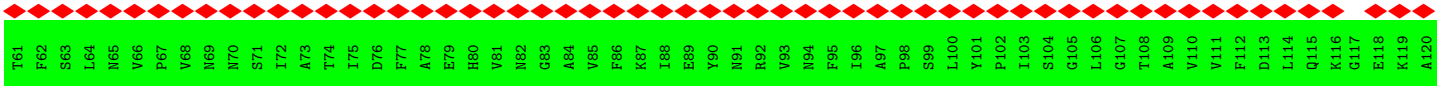


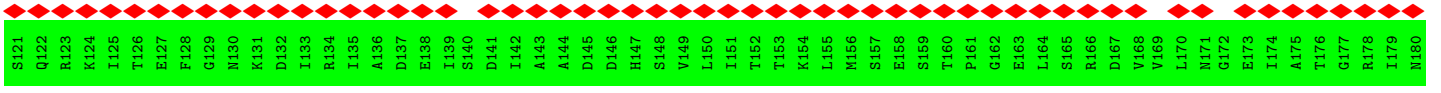


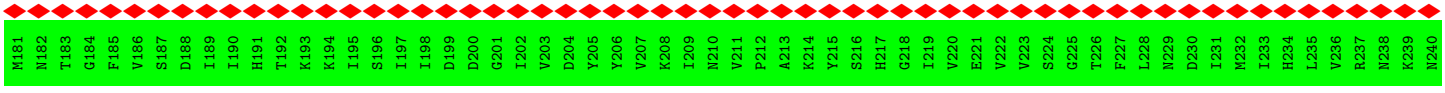
• Molecule 21: P19

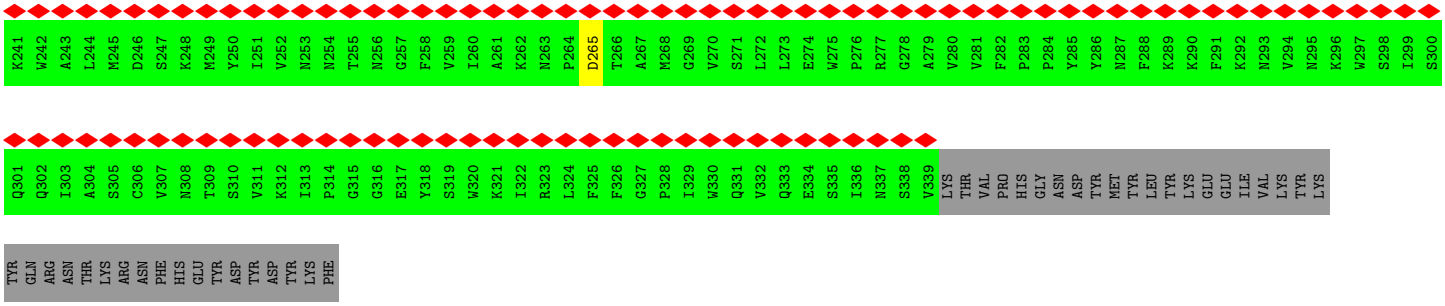
Chain cr:











• Molecule 21: P19

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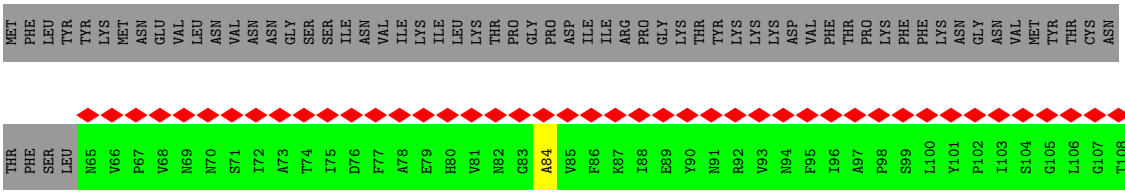

• Molecule 21: P19

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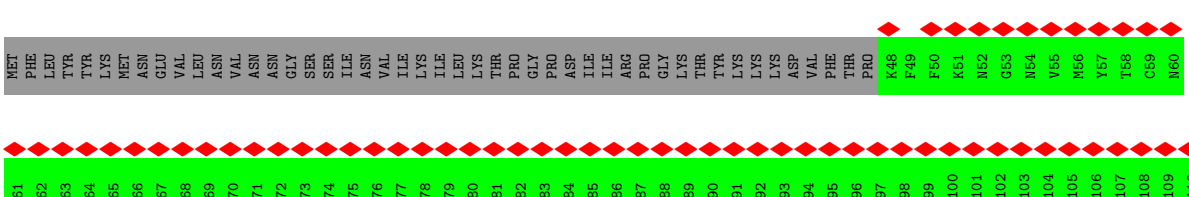

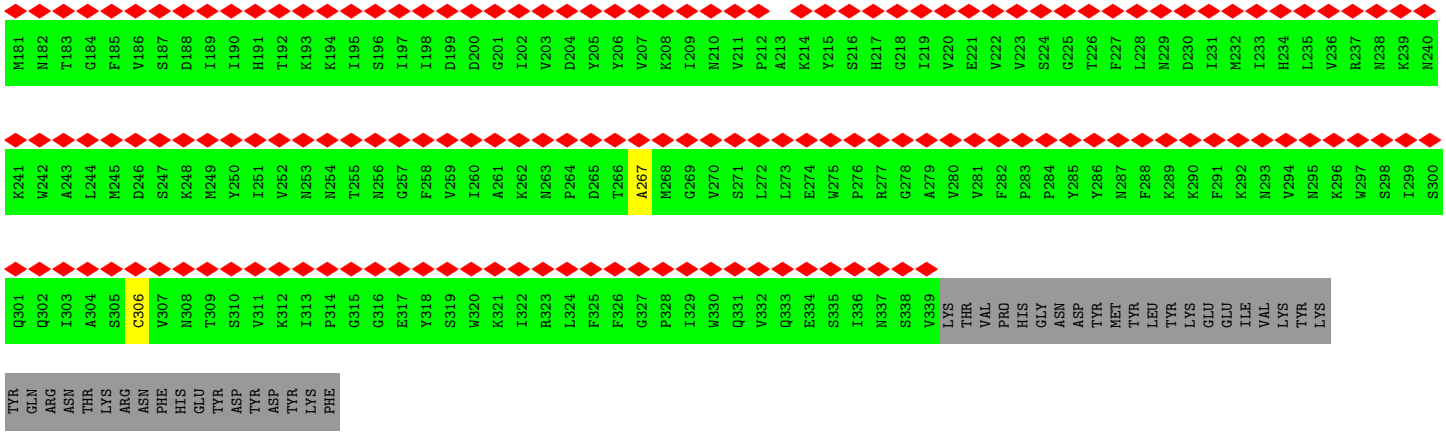

• Molecule 21: P19

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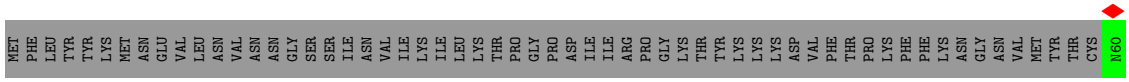

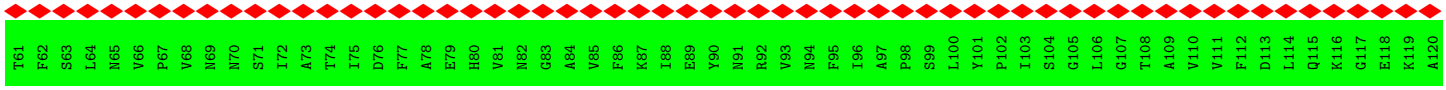

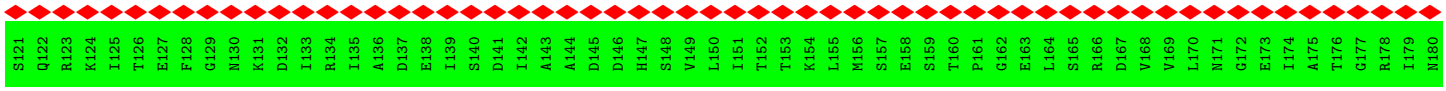

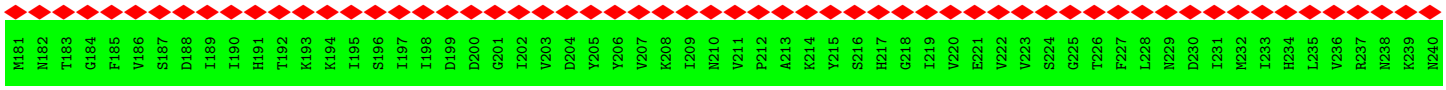

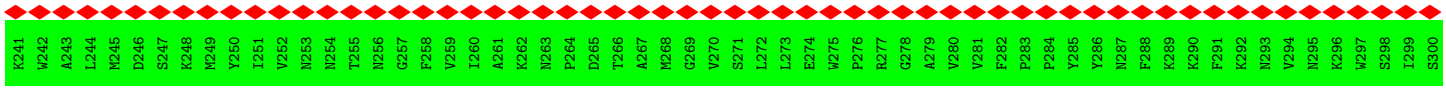

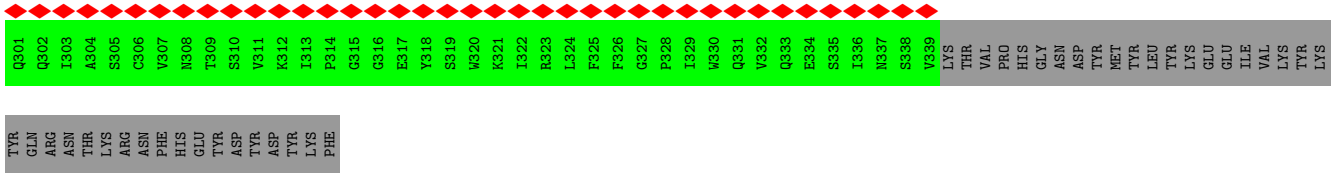

• Molecule 21: P19

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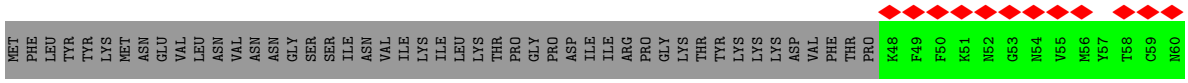

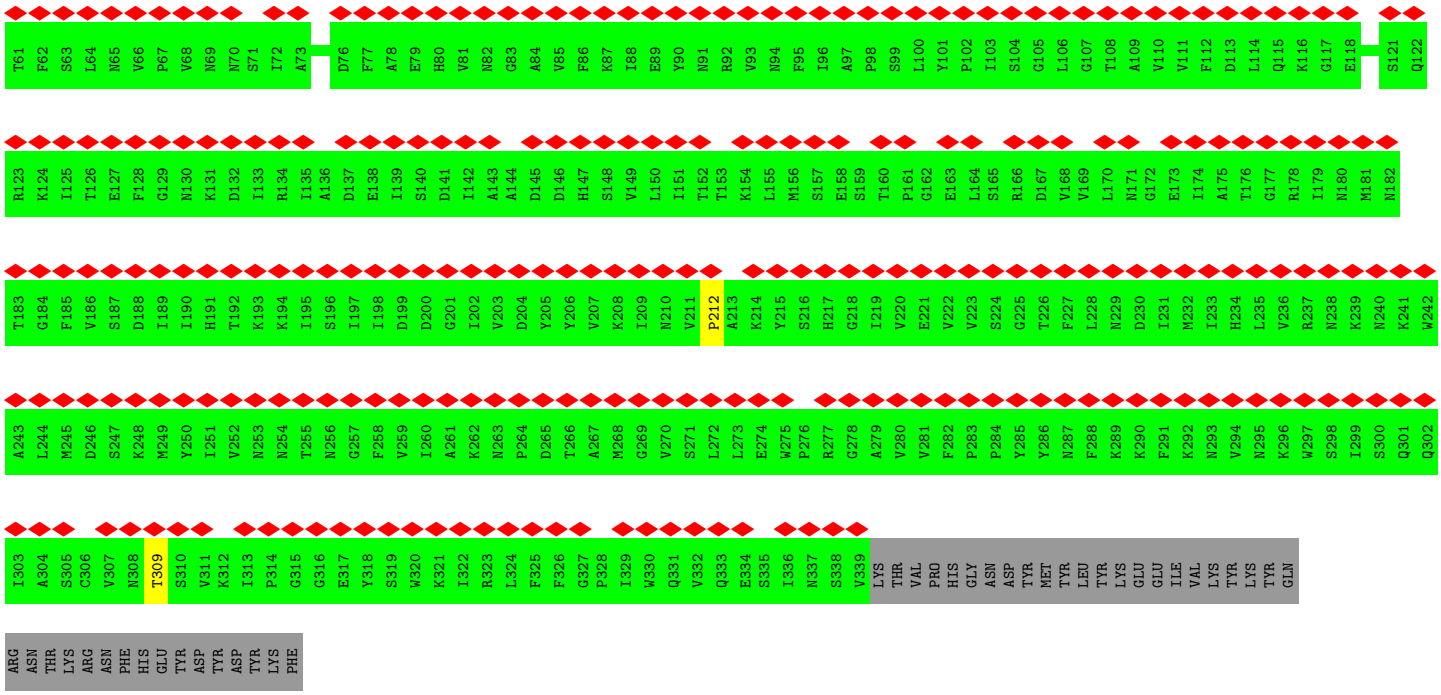

• Molecule 21: P19

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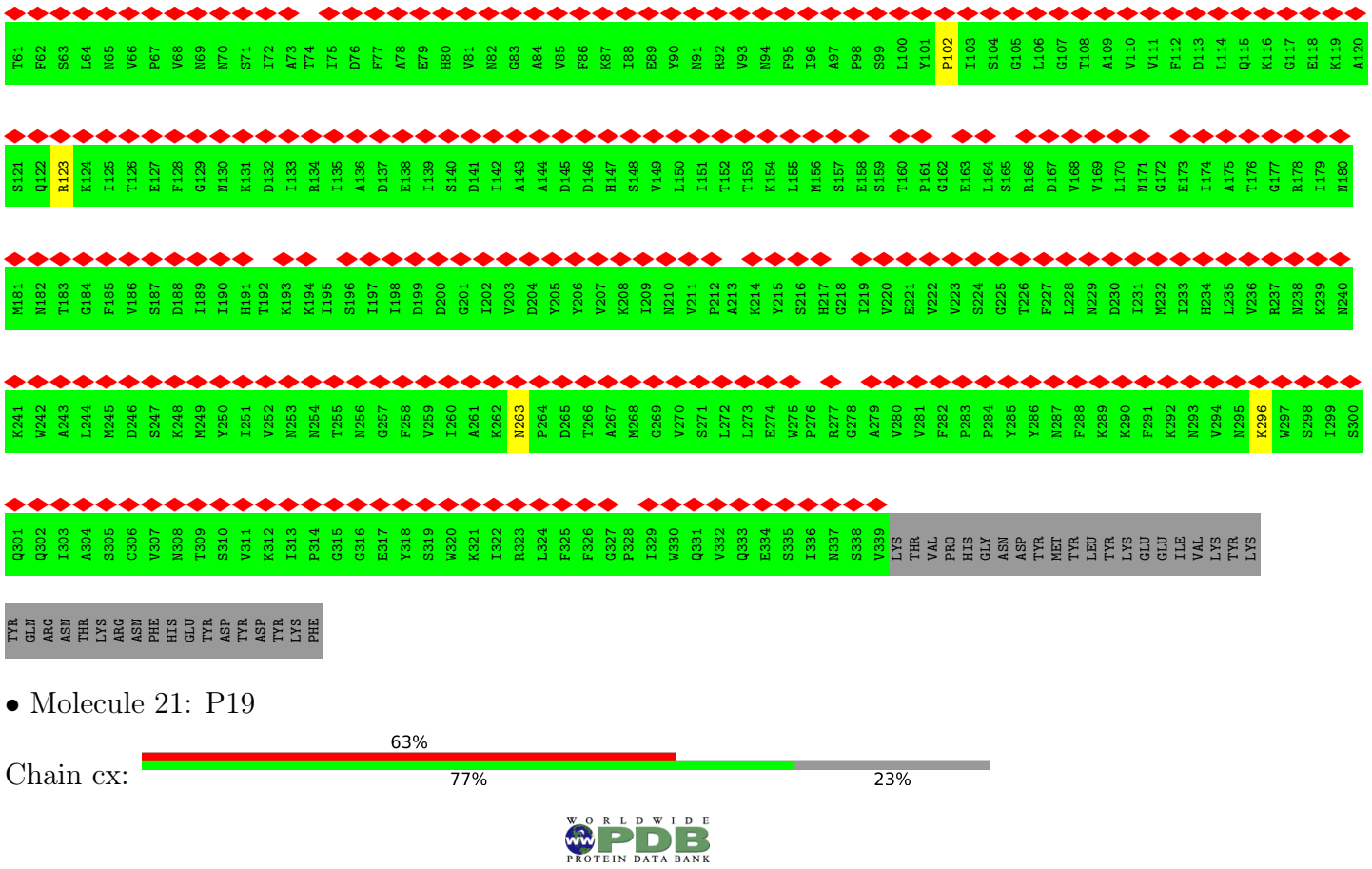

• Molecule 21: P19

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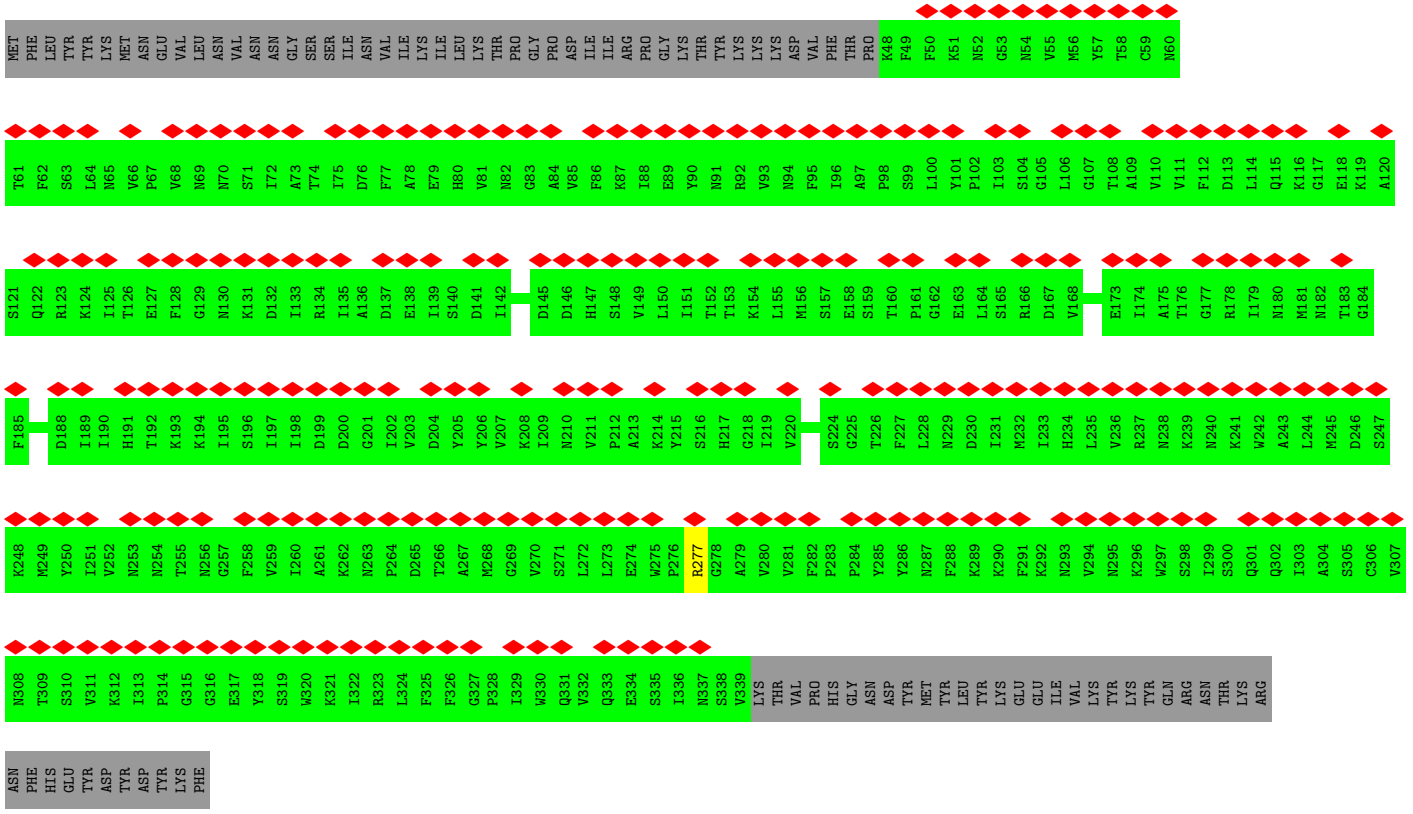
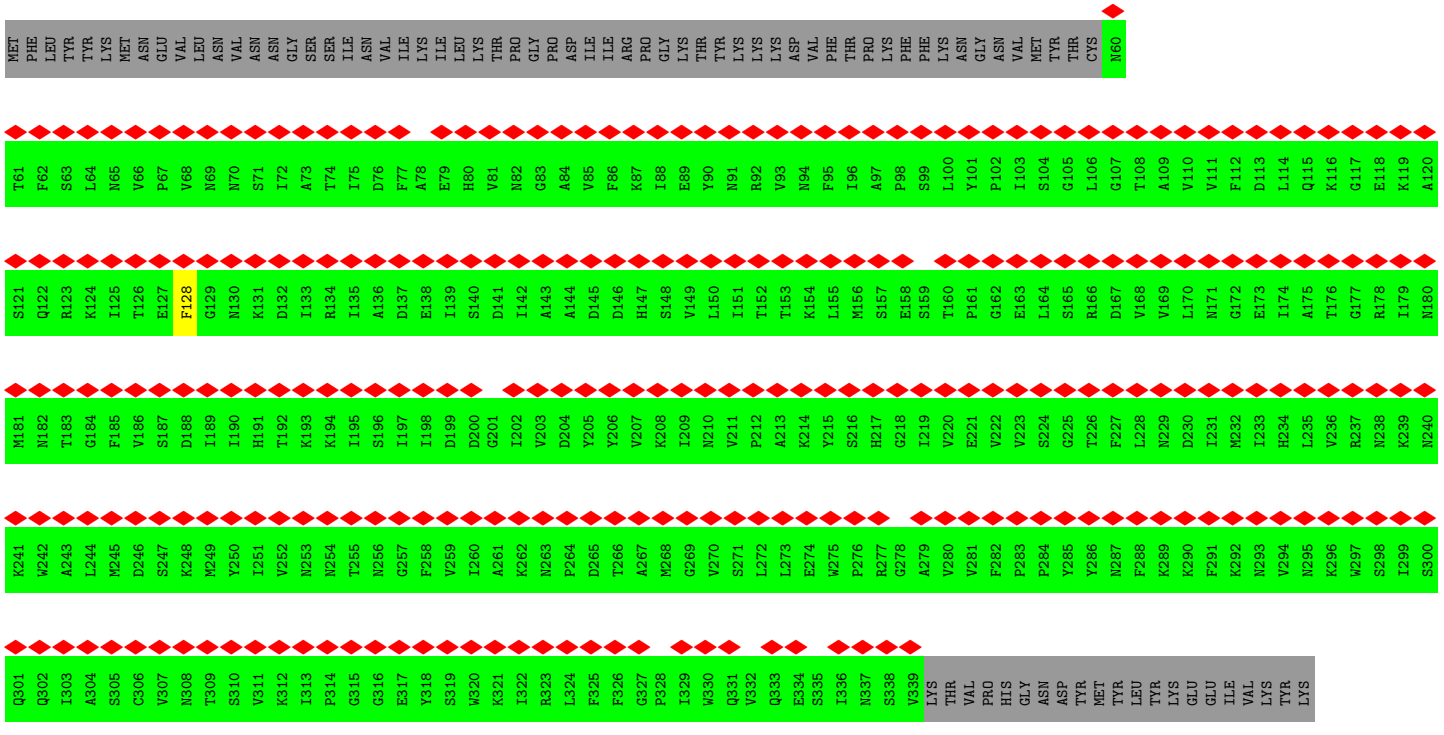


- Molecule 21: P19

Chain cy:



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

• Molecule 21: P19

Chain cz:

MET PHE LEU TYR TYR LYS MET ASN GLU VAL LEU ASN VAL ASN ASN GLY SER SER ILE ASN VAL ILE LYS ILE LEU LYS THR PRO GLY PRO ASP ILE ILE ARG PRO GLY LYS THR TYR LYS LYS ASP VAL PHE THR PRO K48 F49 F50 K51 N52 G53 N54 V55 M56 Y57 T58 C59 N60

T61 F62 S63 L64 N65 V66 P67 V68 N69 N70 S71 I72 A73 T74 I75 D76 F77 A78 E79 H80 V81 N82 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 A109 V110 V111 F112 D113 L114 Q115 K116 G117 E118 K119 A120

S121 Q122 R123 K124 I125 T126 E127 F128 G129 N130 K131 D132 I133 R134 I135 A136 D137 E138 I139 S140 D141 I142 A143 A144 D145 D146 H147 S148 V149 L150 I151 T152 T153 K154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 S165 R166 D167 V168 V169 L170 N171 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 W242 A243 L244 M245 D246 S247 K248 M249 Y250 I251 V252 N253 N254 T255 N256 G257 F258 V259 I260 A261 K262 N263 P264 D265 T266 A267 M268 G269 V270 S271 L272 L273 E274 W275 P276 R277 G278 A279 V280 V281 F282 P283 P284 Y285 Y286 N287 F288 K289 K290 F291 K292 N293 V294 N295 K296 W297 S298 I299 S300

Q301 Q302 I303 A304 S305 C306 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 E334 S335 I336 N337 S338 V339 LYS THR VAL PRO HIS GLY ASN ASP TYR MET TYR LEU TYR LYS GLU GLU ILE VAL LYS TYR LYS

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

• Molecule 21: P19

Chain cA:

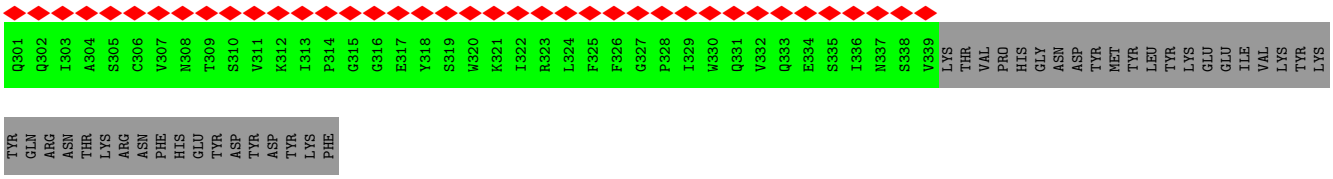
MET PHE LEU TYR TYR LYS MET ASN GLU VAL LEU ASN VAL ASN ASN GLY SER SER ILE ASN VAL ILE LYS ILE LEU LYS THR PRO GLY PRO ASP ILE ILE ARG PRO GLY LYS THR TYR LYS LYS ASP VAL PHE THR PRO LYS PHE PHE LYS ASN GLY ASN VAL MET TYR THR CYS ASN

T61 F62 S63 L64 N65 V66 P67 V68 N69 N70 S71 I72 A73 T74 I75 D76 F77 A78 E79 H80 V81 N82 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 A109 V110 V111 F112 D113 L114 Q115 K116 G117 E118 K119 A120

S121 Q122 R123 K124 I125 T126 E127 F128 G129 N130 K131 D132 I133 R134 I135 A136 D137 E138 I139 S140 D141 I142 A143 A144 D145 D146 H147 S148 V149 L150 I151 T152 T153 K154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 S165 R166 D167 V168 V169 L170 N171 G172 E173 I174 A175 T176 G177 R178 I179 N180

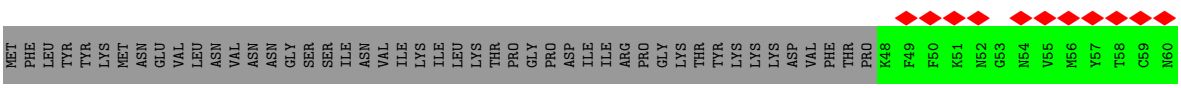
M181 N182 T183 G184 F185 V186 S187 D188 I189 I190 H191 T192 K193 K194 I195 S196 I197 I198 D199 D200 G201 I202 V203 D204 Y205 Y206 V207 K208 I209 N210 V211 P212 A213 K214 Y215 S216 H217 G218 I219 V220 E221 V222 V223 S224 G225 T226 F227 L228 N229 D230 I231 M232 I233 H234 L235 V236 R237 N238 K239 N240

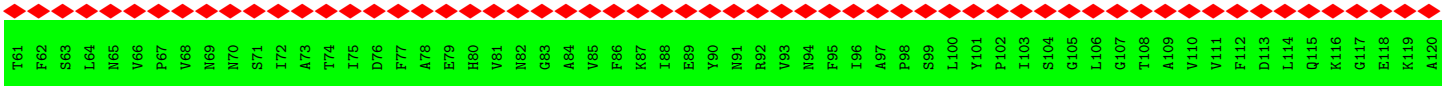
K241 W242 A243 L244 M245 D246 S247 K248 M249 Y250 I251 V252 N253 N254 T255 N256 G257 F258 V259 I260 A261 K262 N263 P264 D265 T266 A267 M268 G269 V270 S271 L272 L273 E274 W275 P276 R277 G278 A279 V280 V281 F282 P283 P284 Y285 Y286 N287 F288 K289 K290 F291 K292 N293 V294 N295 K296 W297 S298 I299 S300

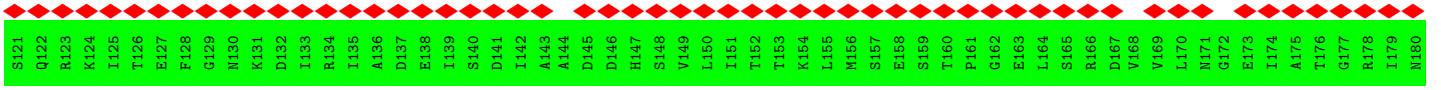


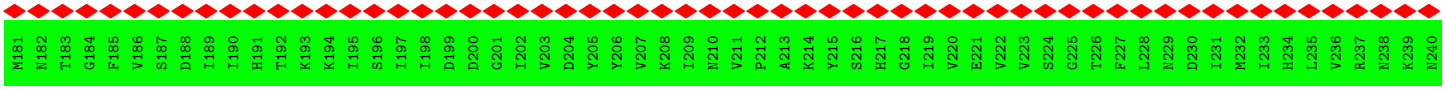
• Molecule 21: P19

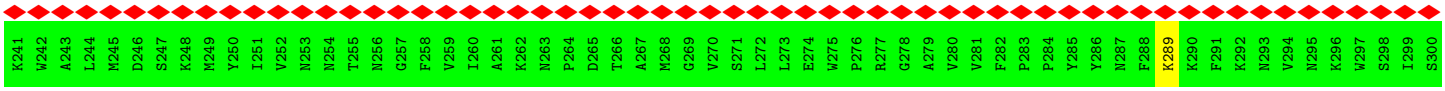
Chain cB:

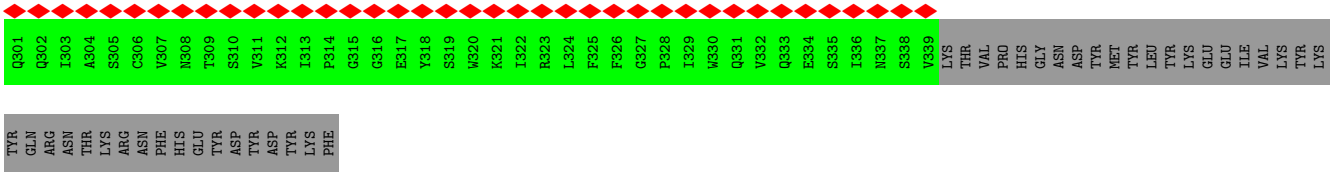






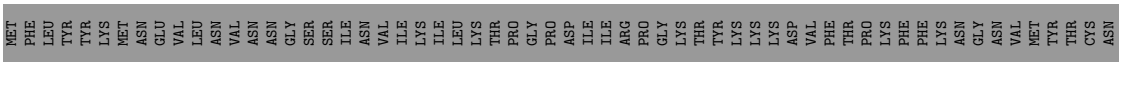


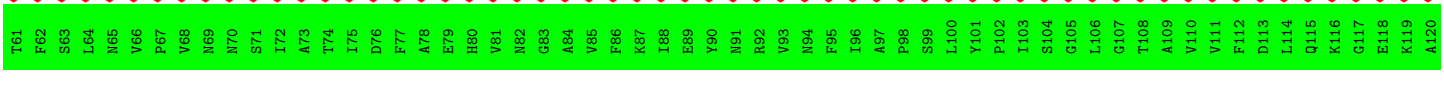


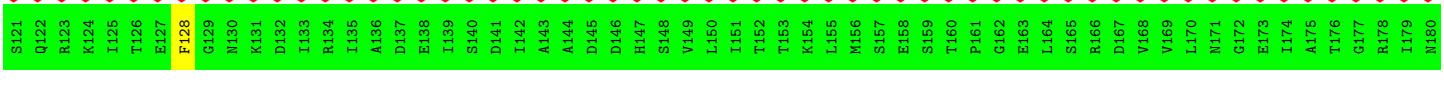


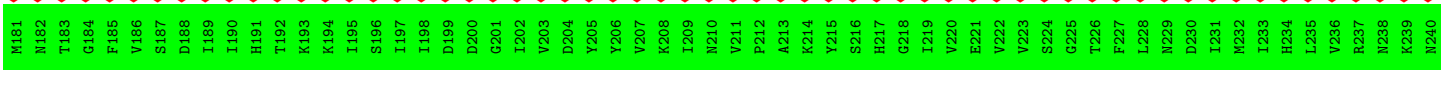
• Molecule 21: P19

Chain cC:









• Molecule 21: P19

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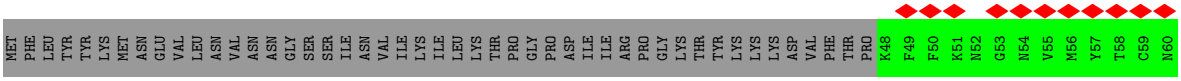
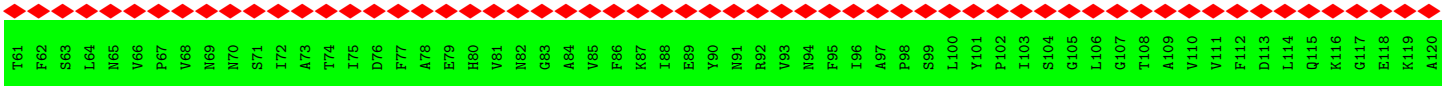
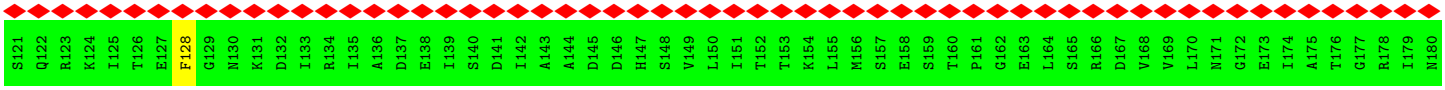
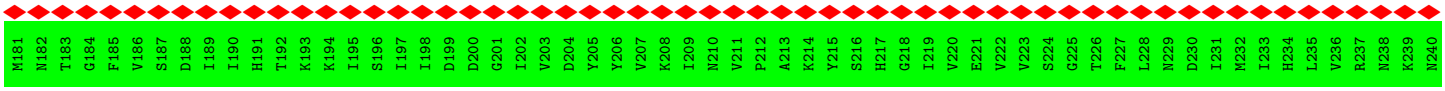
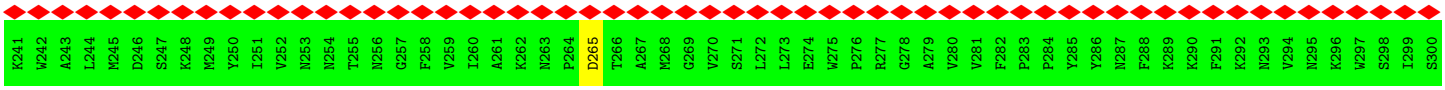
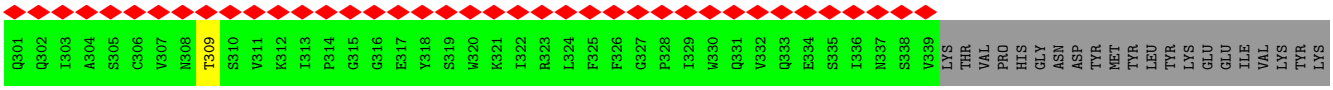






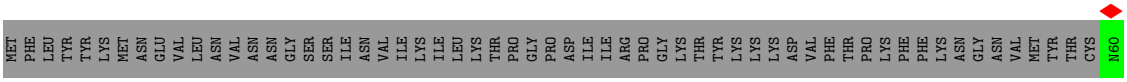


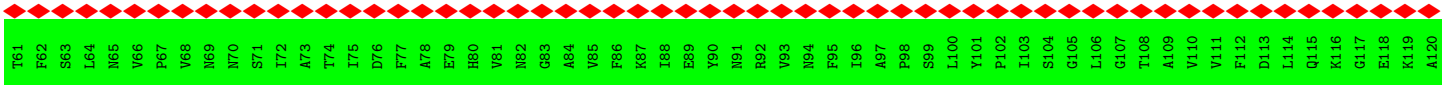




• Molecule 21: P19

Chain cE:





• Molecule 21: P19

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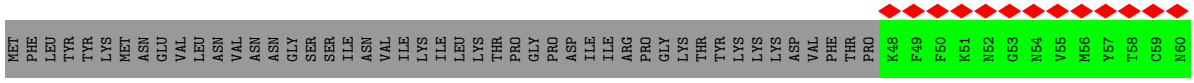

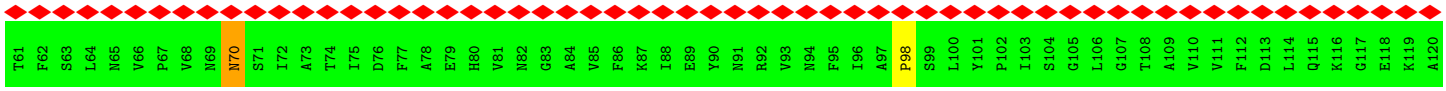

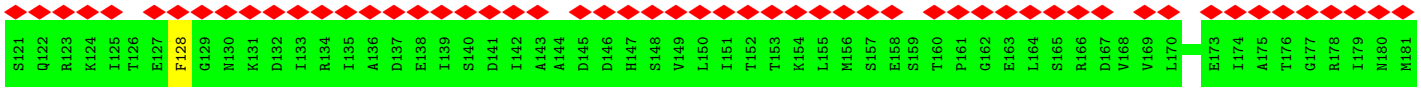

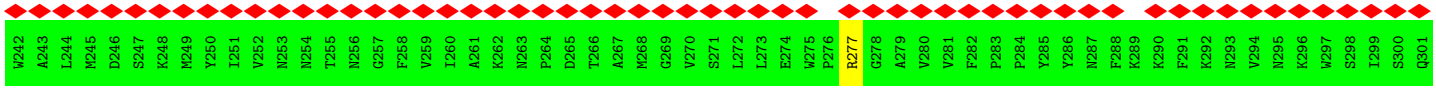

• Molecule 21: P19

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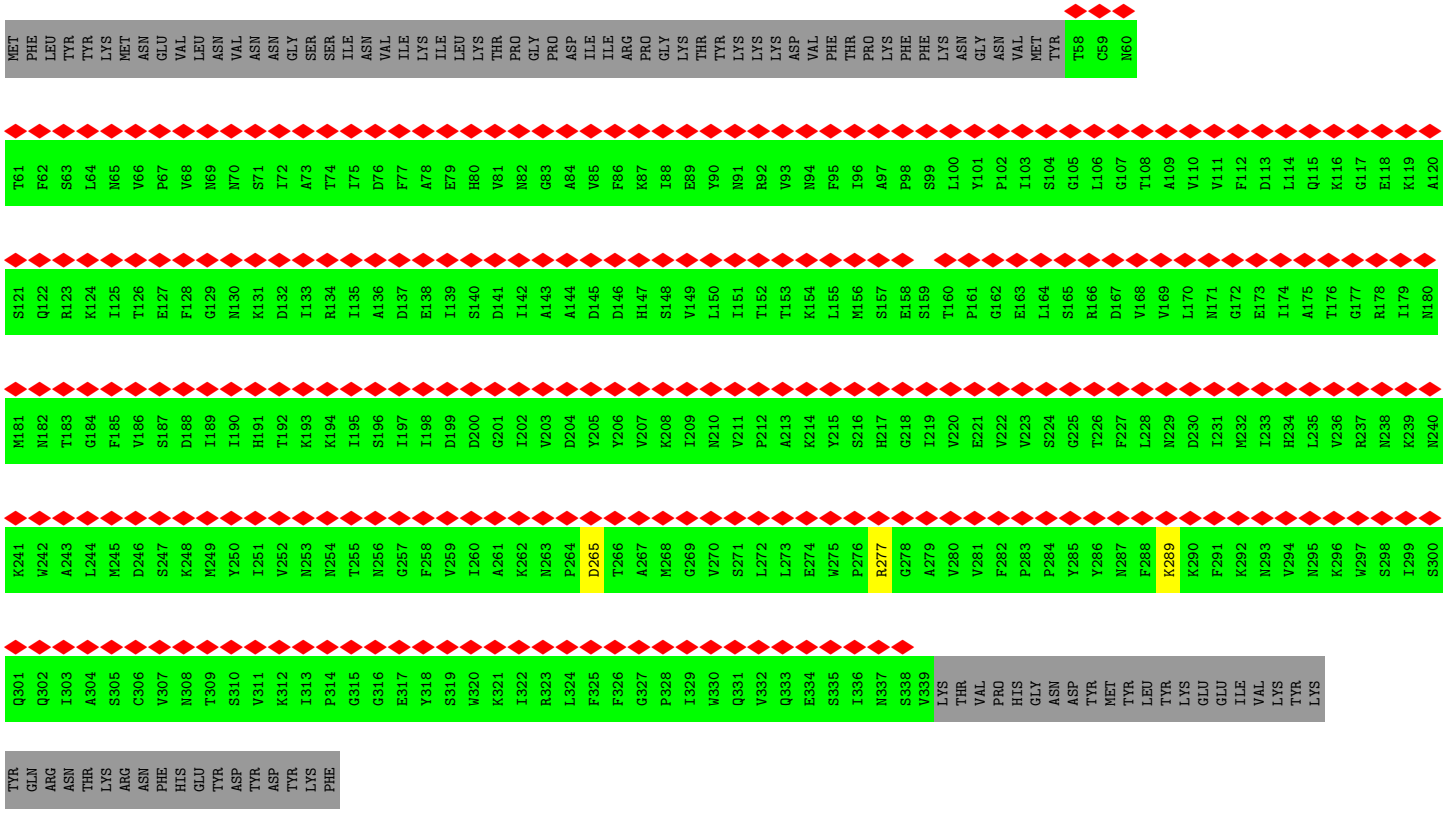
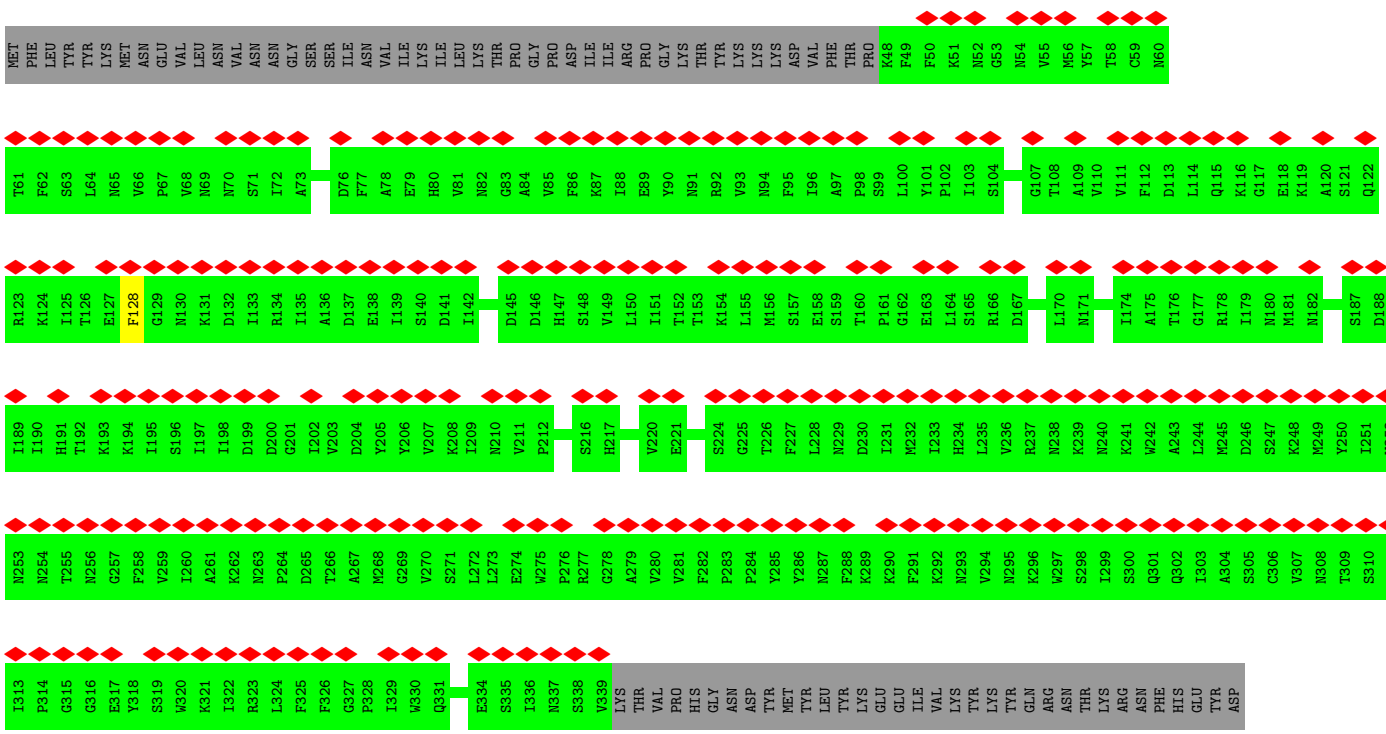


• Molecule 21: P19

Chain cH:



TYR ASP TYR LYS PHE

• Molecule 21: P19

Chain cI:

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

T61 F62 S63 L64 N65 V66 P67 V68 N69 N70 S71 I72 A73 T74 I75 D76 F77 A78 E79 H80 V81 N82 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 A109 V110 V111 F112 D113 L114 Q115 K116 G117 E118 K119 A120

S121 Q122 R123 K124 I125 T126 E127 F128 G129 N130 K131 D132 I133 R134 I135 A136 D137 E138 I139 S140 D141 I142 A143 A144 D145 D146 H147 S148 V149 L150 I151 T152 T153 K154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 S165 R166 D167 V168 V169 L170 N171 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 Y222 V223 S224 G225 T226 F227 L228 N229 D230 I231 M232 I233 H234 L235 Y236 R237 N238 K239 N240

K241 W242 A243 L244 M245 D246 S247 K248 M249 Y250 I251 V252 N253 N254 T255 N256 G257 F258 V259 I260 A261 K262 N263 P264 D265 T266 A267 M268 G269 V270 S271 L272 L273 E274 W275 P276 R277 G278 A279 V280 V281 F282 P283 P284 Y285 Y286 N287 F288 K289 K290 F291 K292 N293 V294 N295 K296 W297 S298 I299 S300

Q301 Q302 I303 A304 S305 C306 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 E334 S335 I336 N337 S338 V339 LYS THR VAL PRO HIS GLY ASN ASP TYR MET TYR LEU TYR LYS GLU GLU ILE VAL LYS TYR LYS

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

• Molecule 21: P19

Chain cJ:

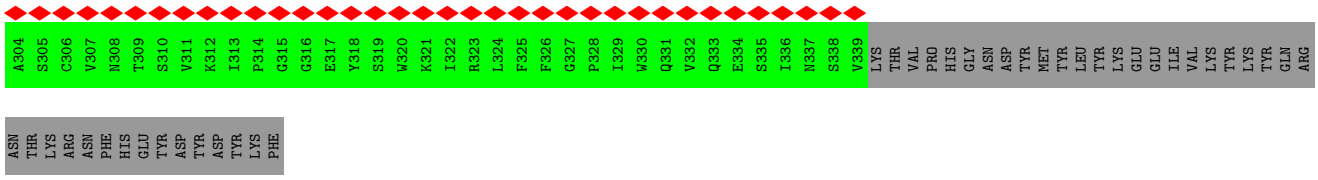
MET PHE LEU TYR TYR LYS MET ASN GLU VAL LEU ASN VAL ASN ASN GLY SER SER ILE ASN VAL ILE LYS ILE LEU LYS THR PRO GLY PRO ASP ILE ILE ARG PRO GLY LYS THR TYR LYS LYS LYS ASP VAL PHE THR PRO K48 F49 F50 K51 N52 G53 N54 V55 M56 Y57 T58 C59 N60

T61 F62 S63 L64 N65 V66 P67 V68 N69 N70 S71 I72 A73 T74 I75 D76 F77 A78 E79 H80 V81 N82 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 A109 V110 V111 F112 D113 L114 Q115 K116 G117 E118 K119 A120

S121 Q122 R123 K124 I125 T126 E127 F128 G129 N130 K131 D132 I133 R134 I135 A136 D137 E138 I139 S140 D141 I142 D145 D146 H147 S148 V149 L150 I151 T152 T153 K154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 S165 R166 D167 V168 V169 L170 N171 I174 A175 T176 G177 R178 I179 N180 M181 N182

T183 G184 F185 V186 S187 D188 I189 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 W242 A243

L244 M245 D246 S247 K248 M249 Y250 I251 V252 N253 N254 T255 N256 G257 F258 V259 I260 A261 K262 N263 P264 D265 T266 A267 M268 G269 V270 S271 L272 L273 E274 W275 P276 R277 G278 A279 V280 V281 F282 P283 P284 Y285 Y286 N287 F288 K289 K290 F291 K292 N293 V294 N295 K296 W297 S298 I299 S300 Q301 Q302 I303



• Molecule 21: P19

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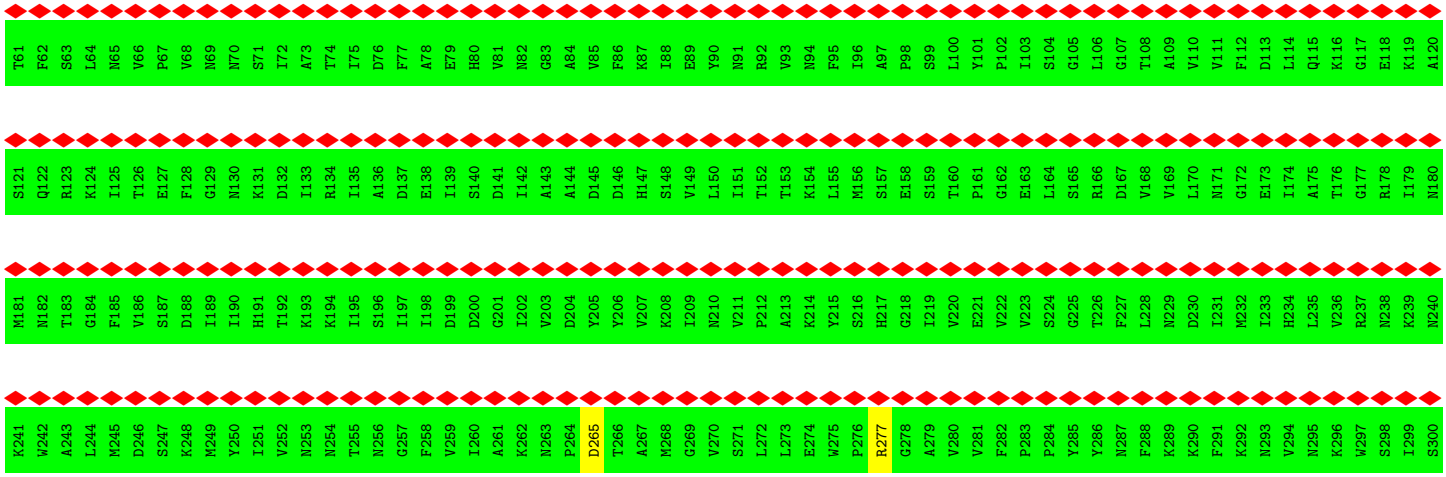
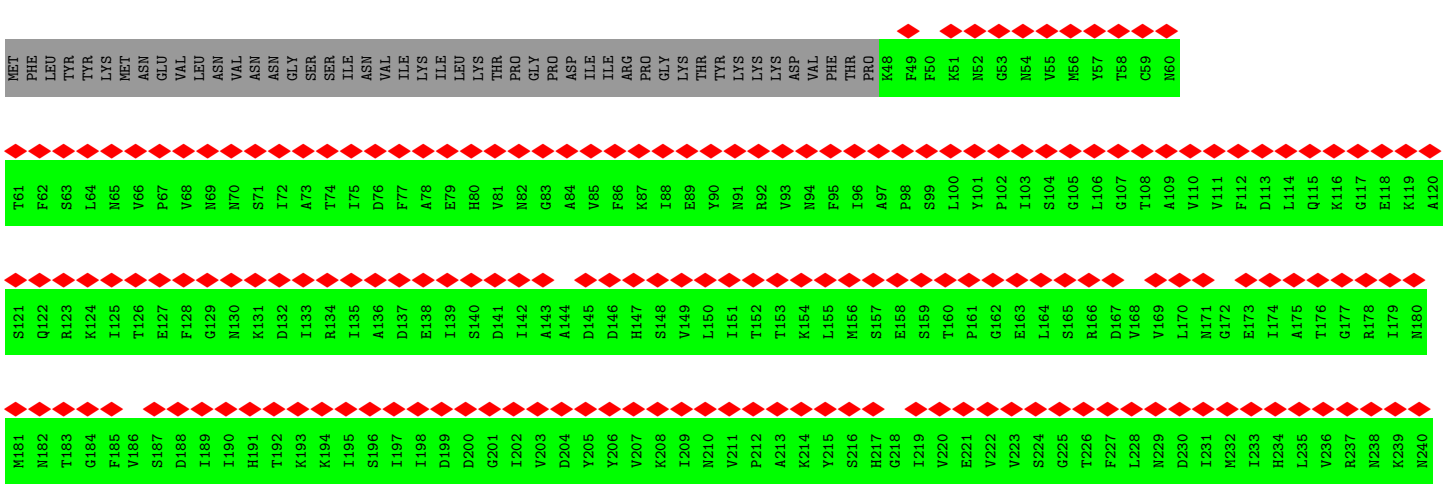
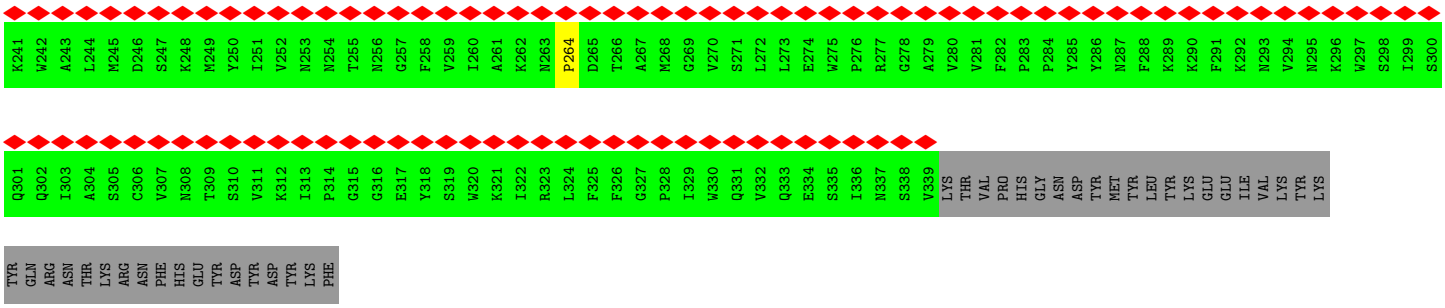


• Molecule 21: P19

Chain cL:





• Molecule 21: P19

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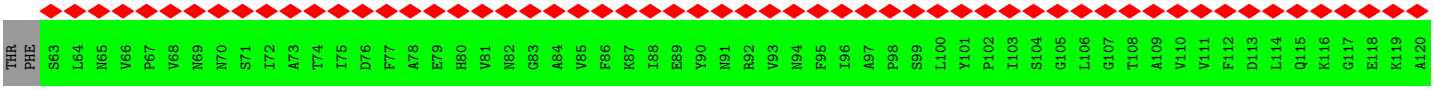
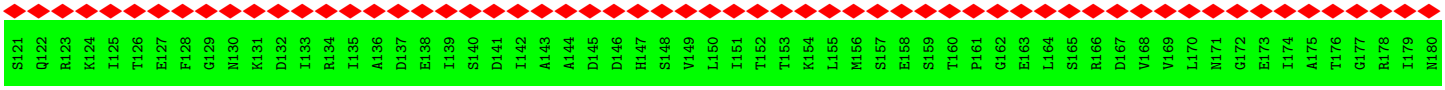
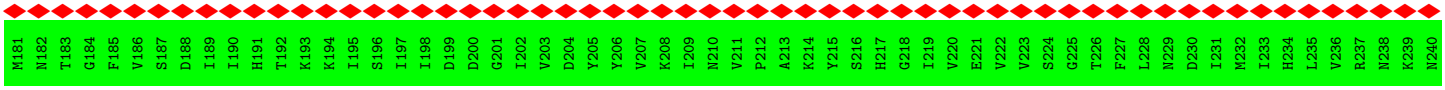
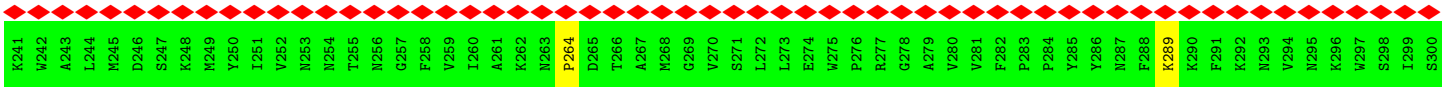
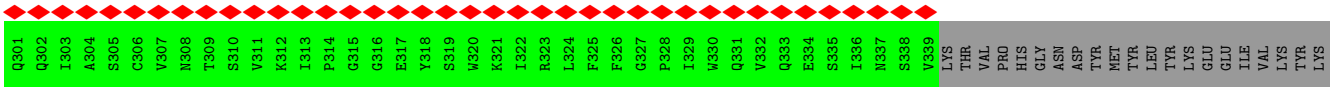




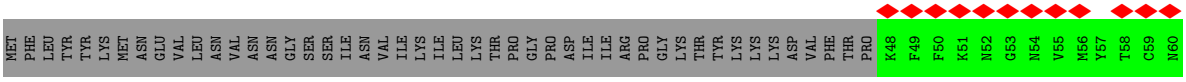


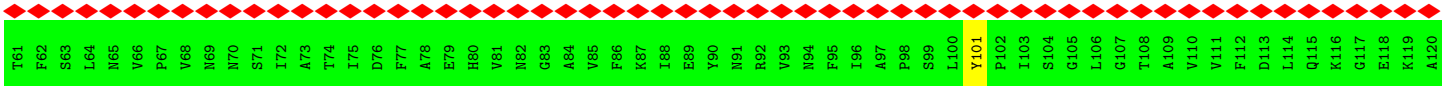


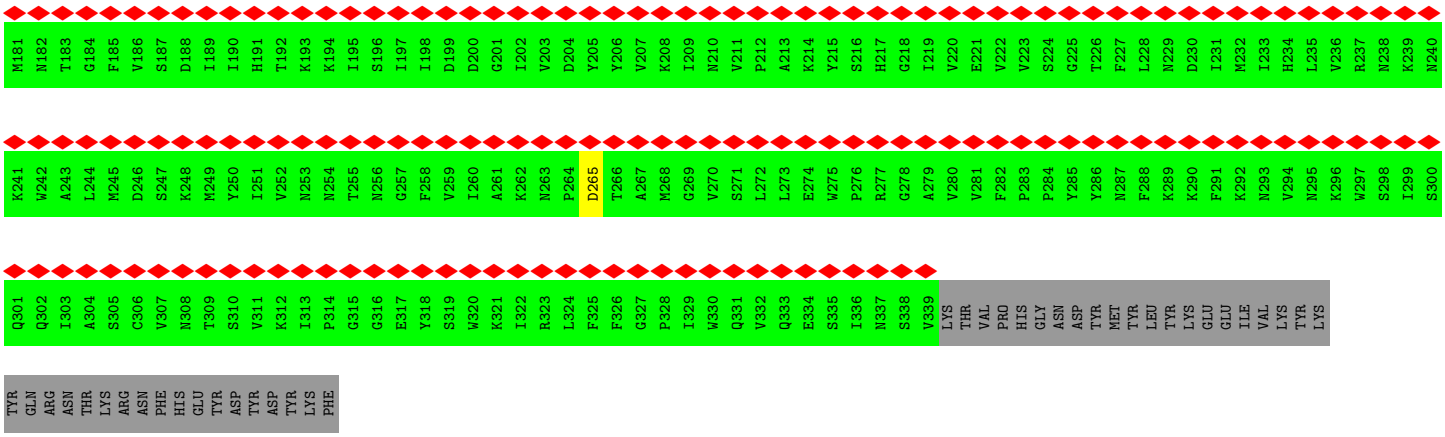


• Molecule 21: P19

Chain cN:

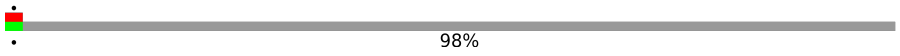


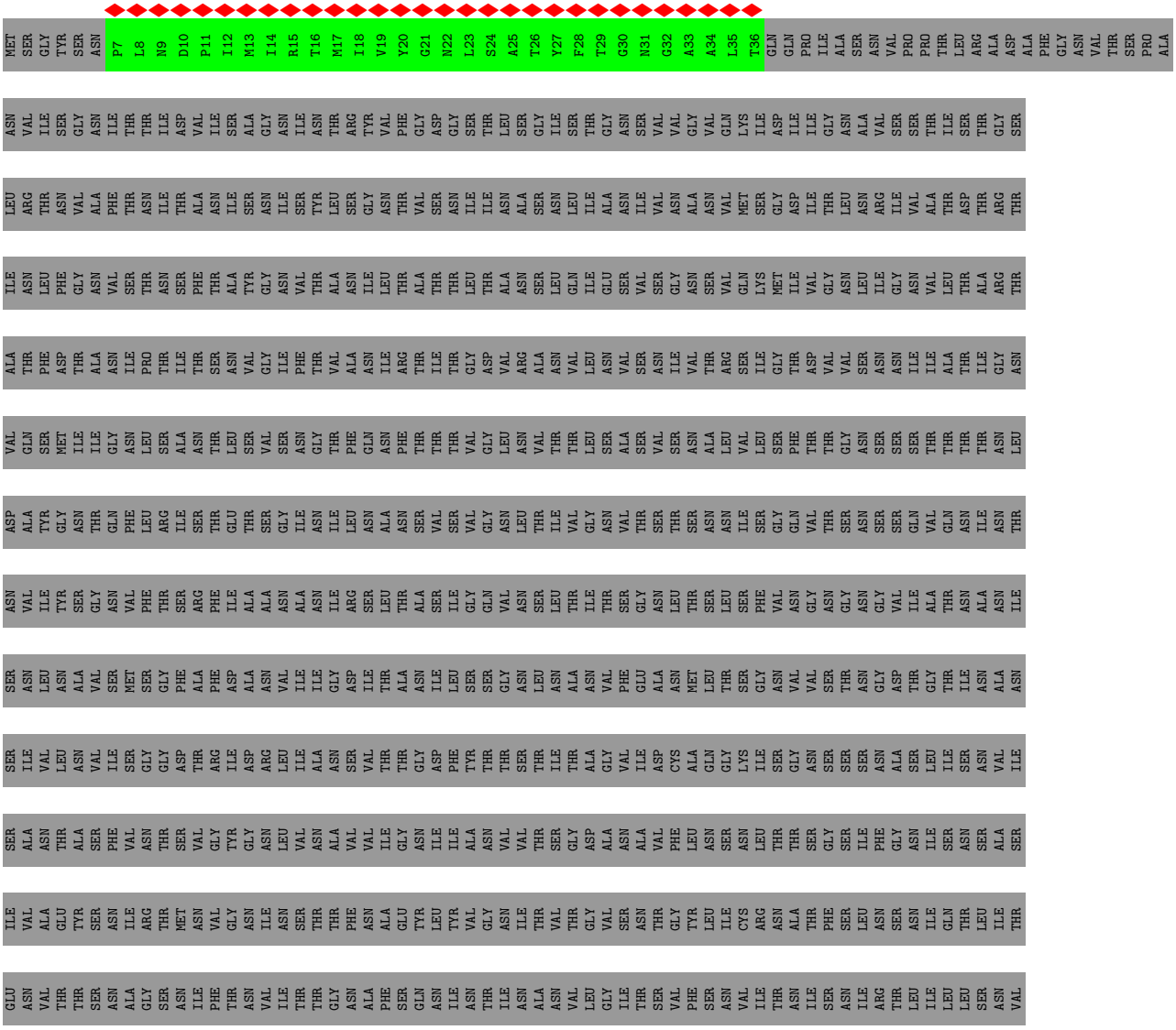


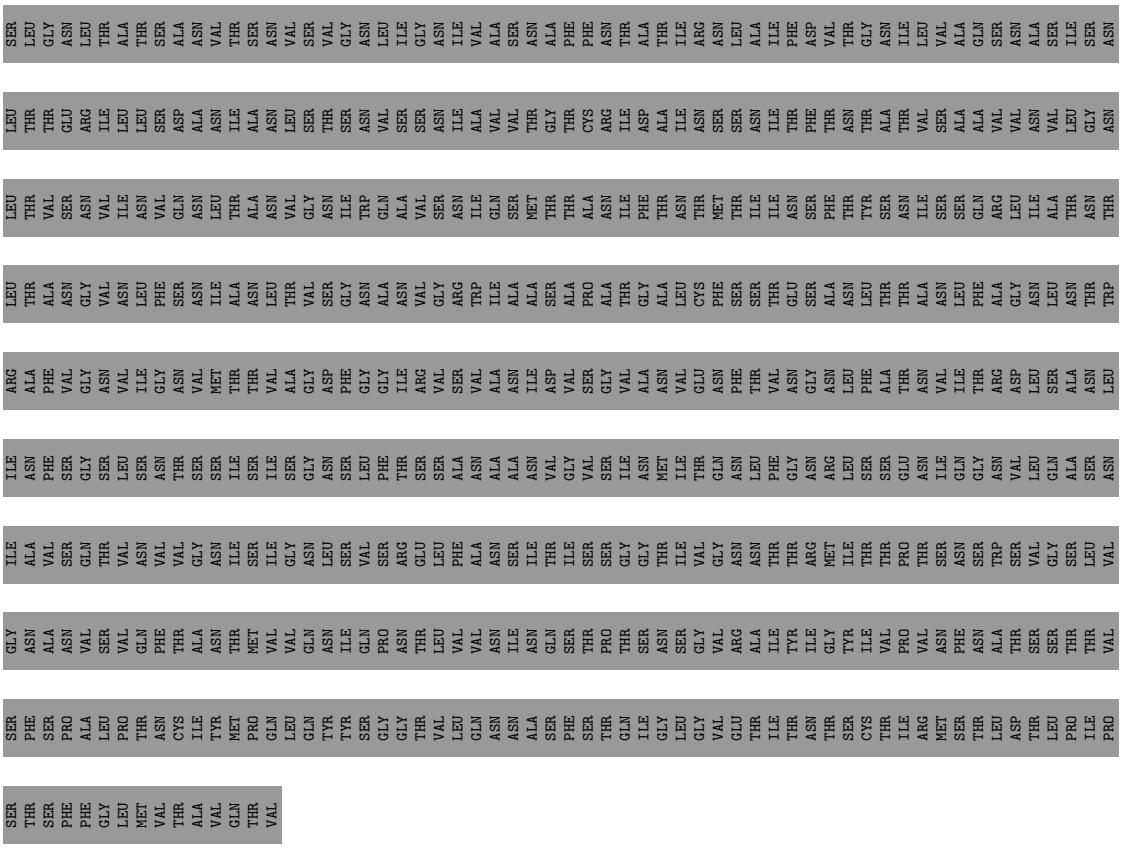


• Molecule 22: P20

Chain cO:







- Molecule 22: P20

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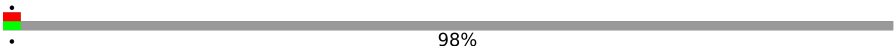
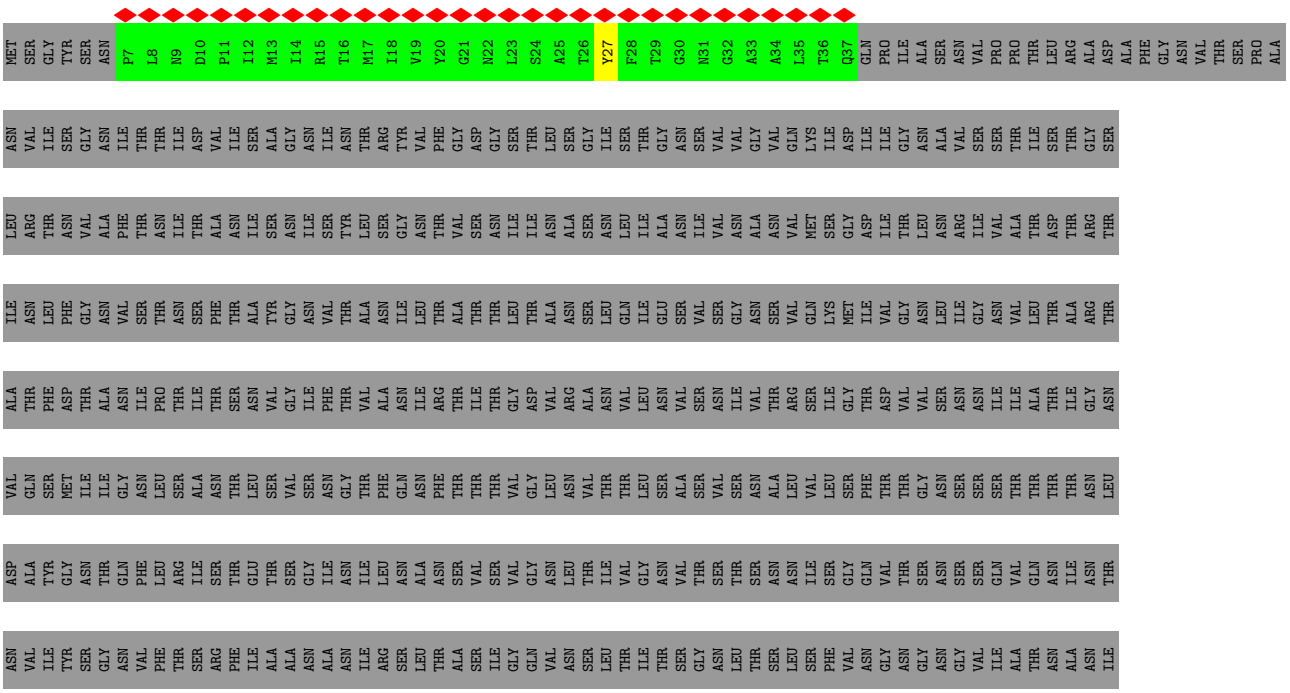
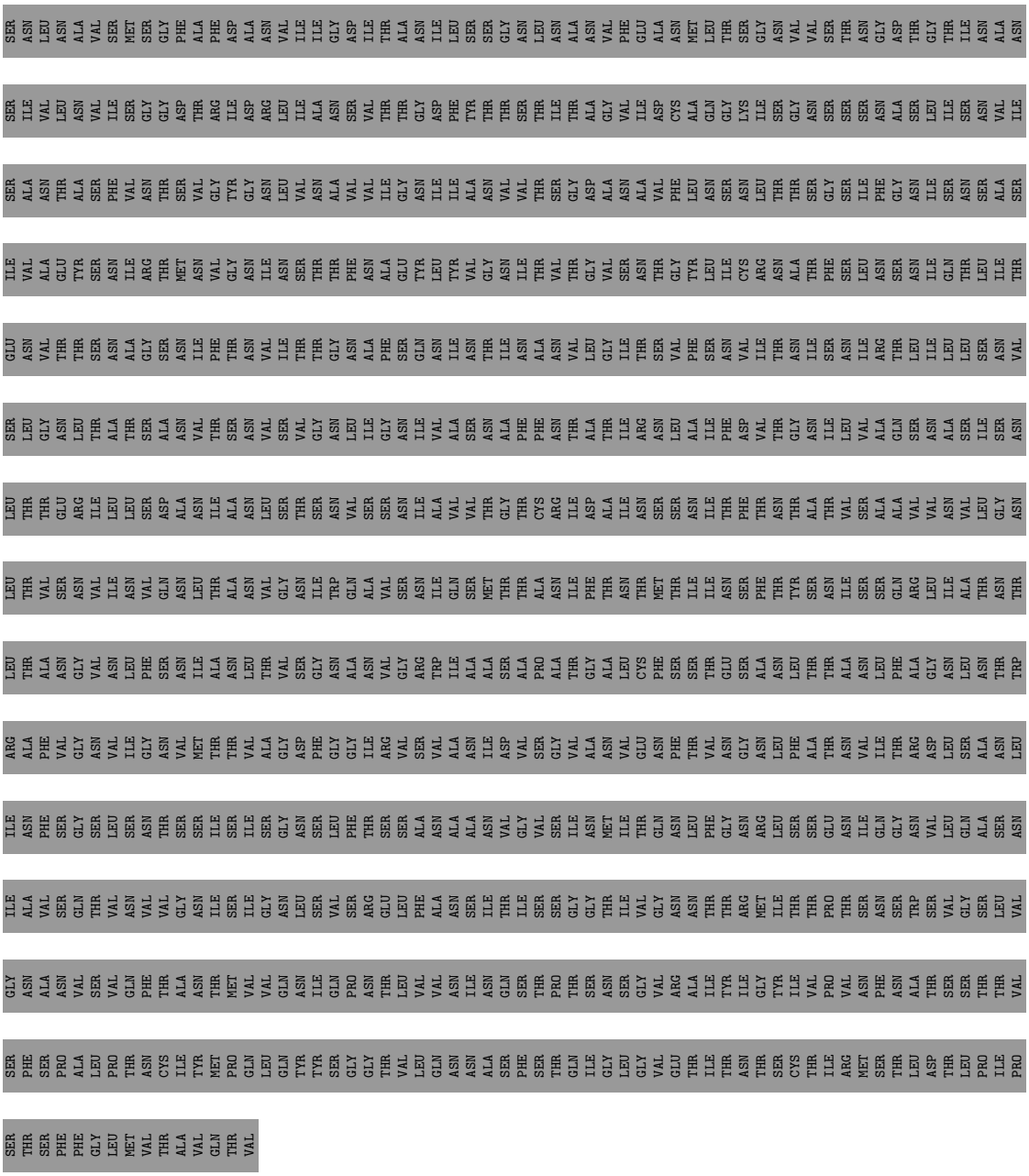
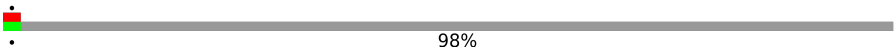


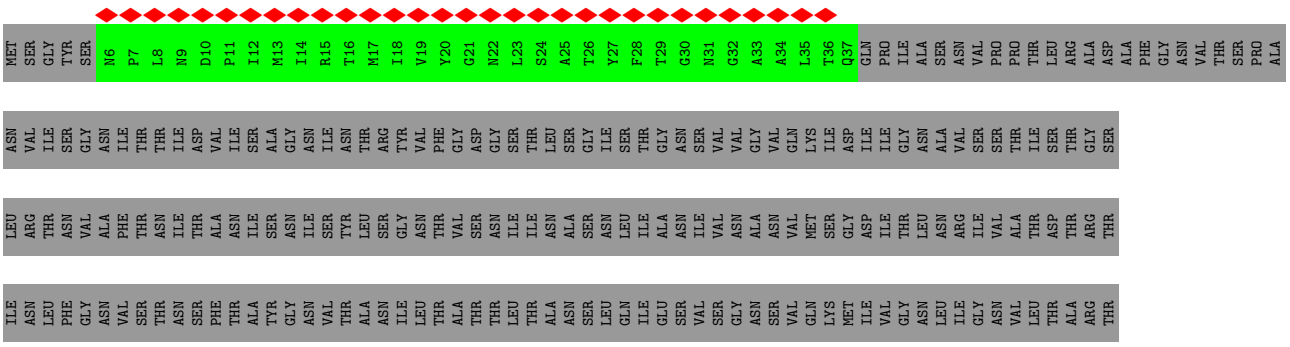


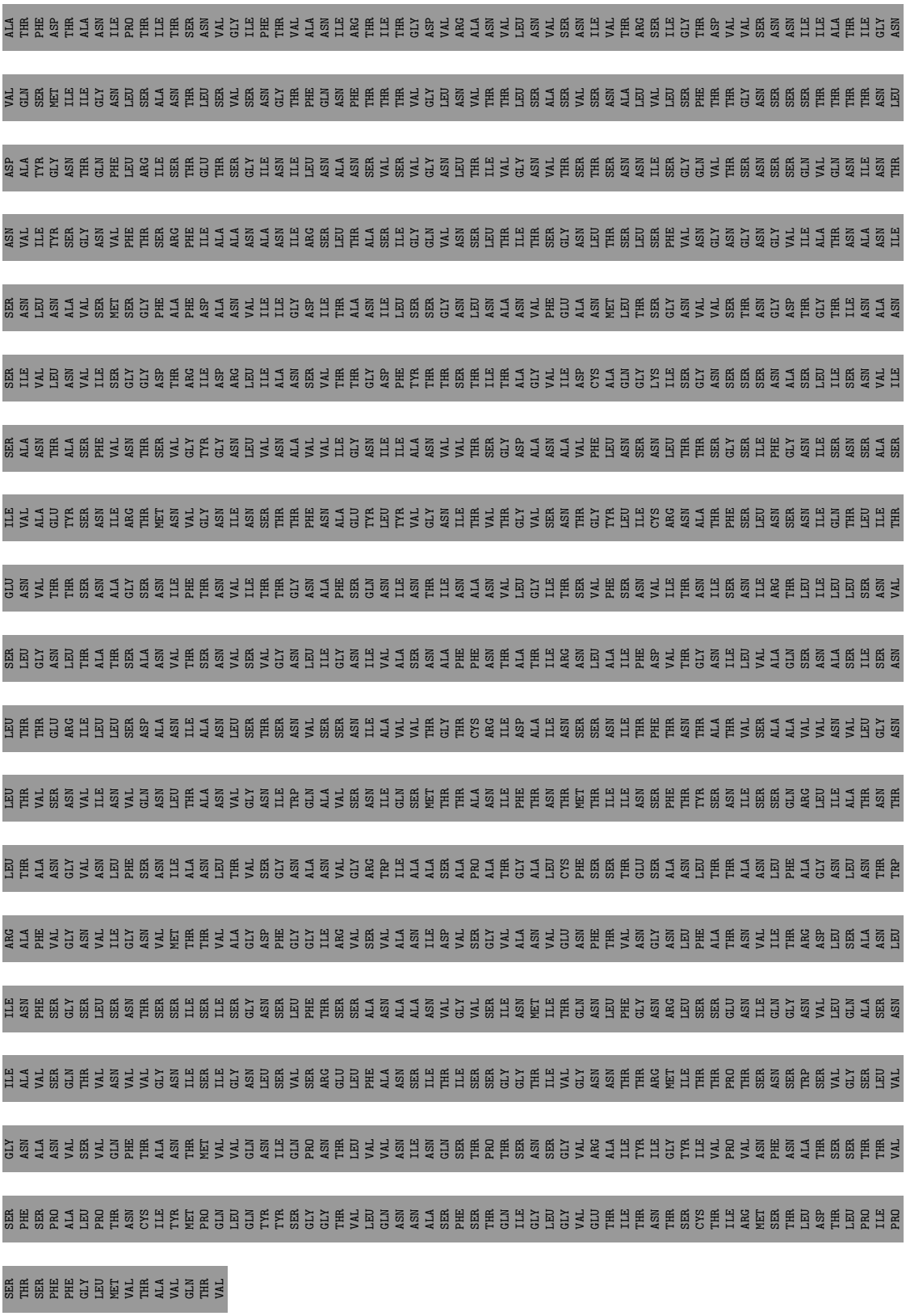


• Molecule 22: P20

Chain da:

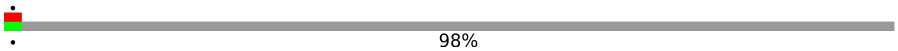


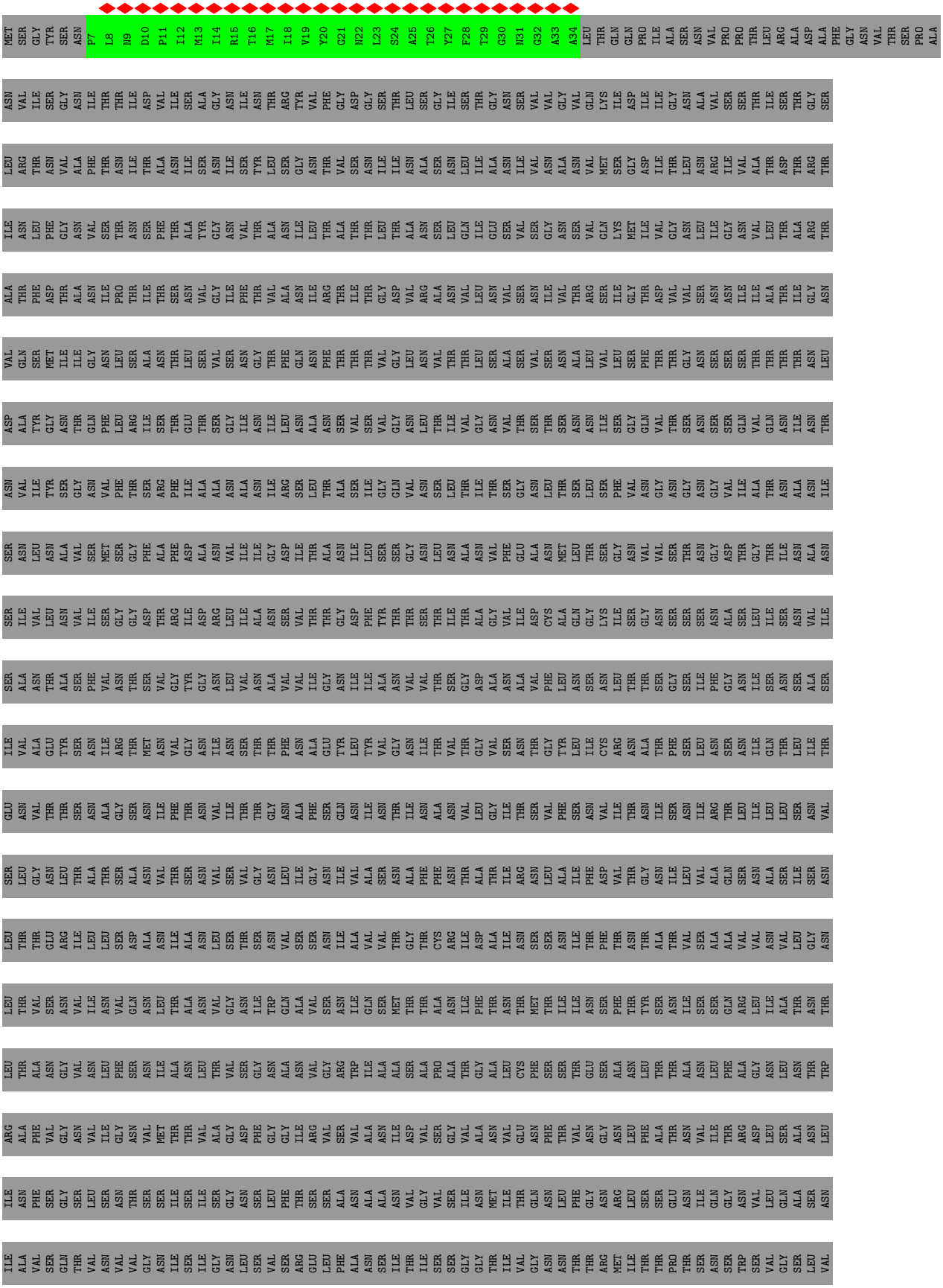




• Molecule 22: P20

Chain dc:

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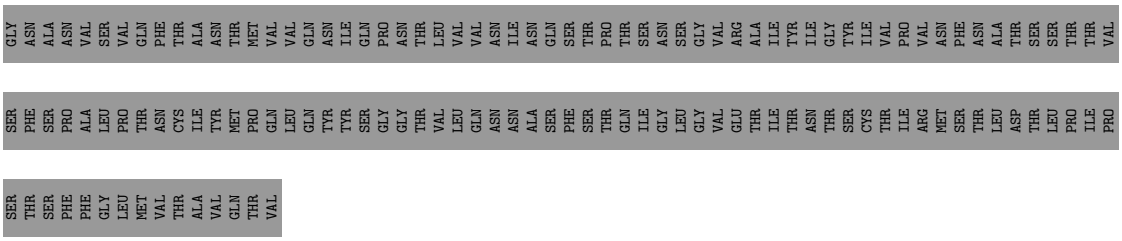
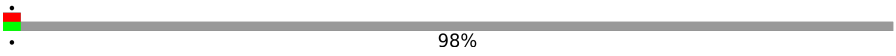
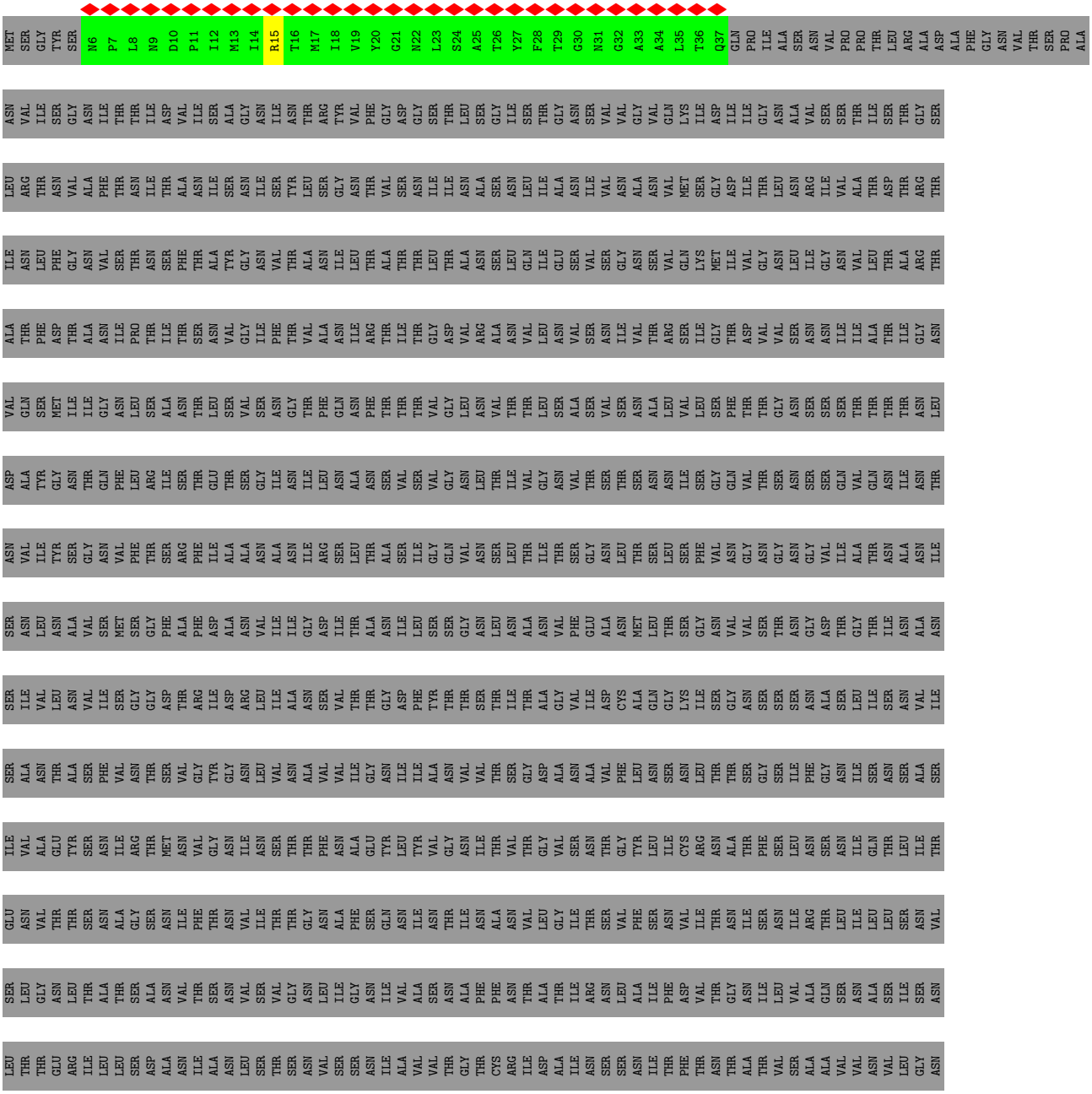
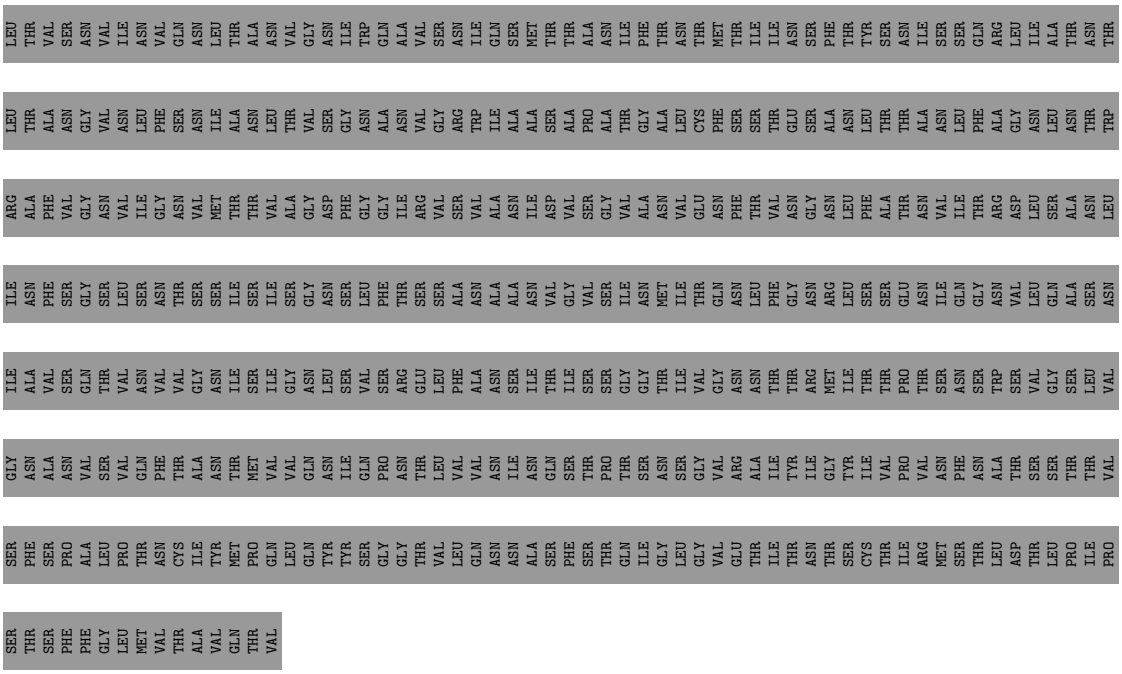


• Molecule 22: P20

Chain dg:







• Molecule 22: P20

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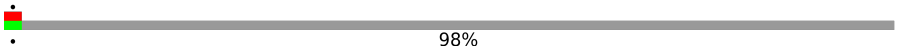

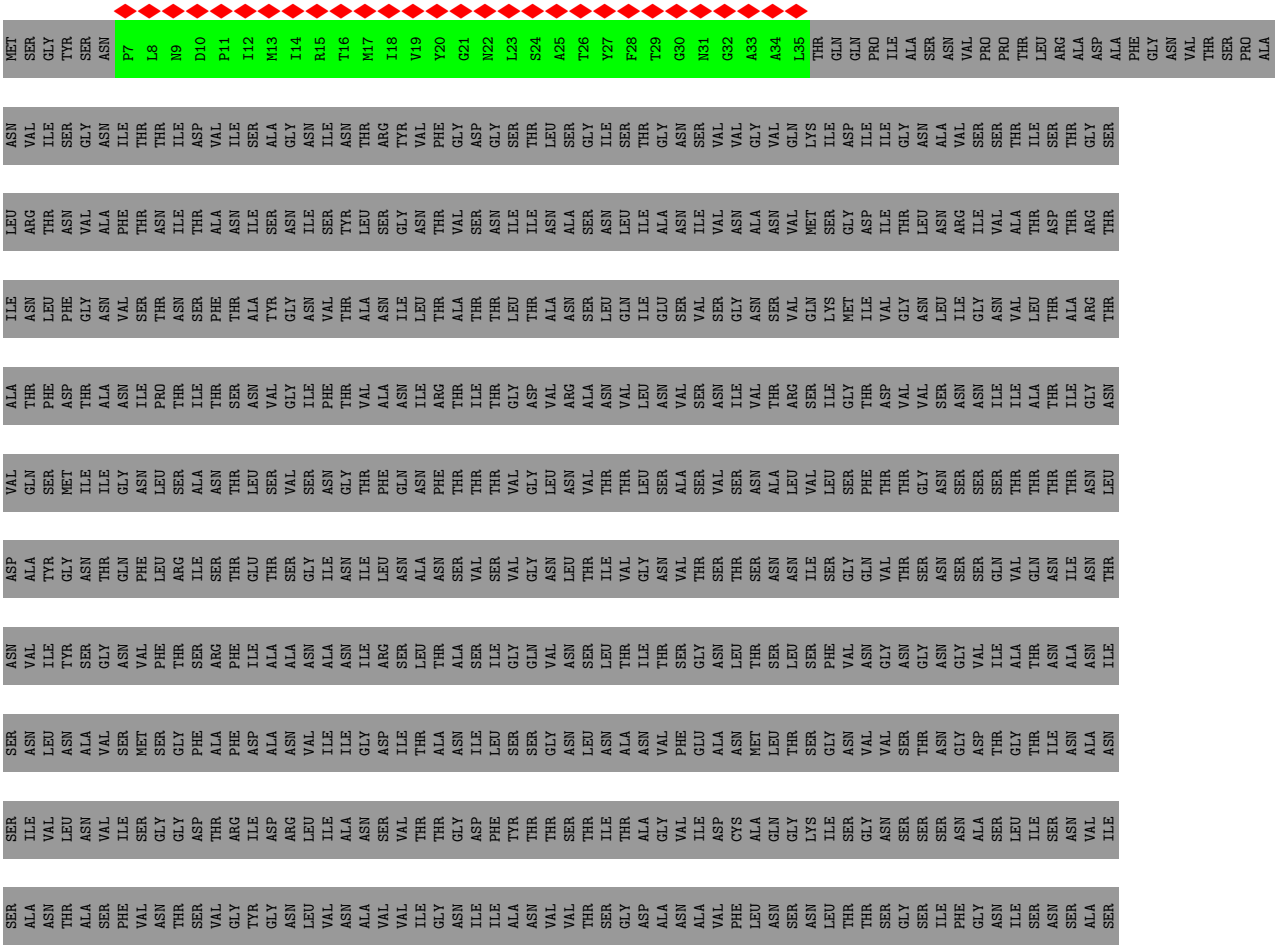

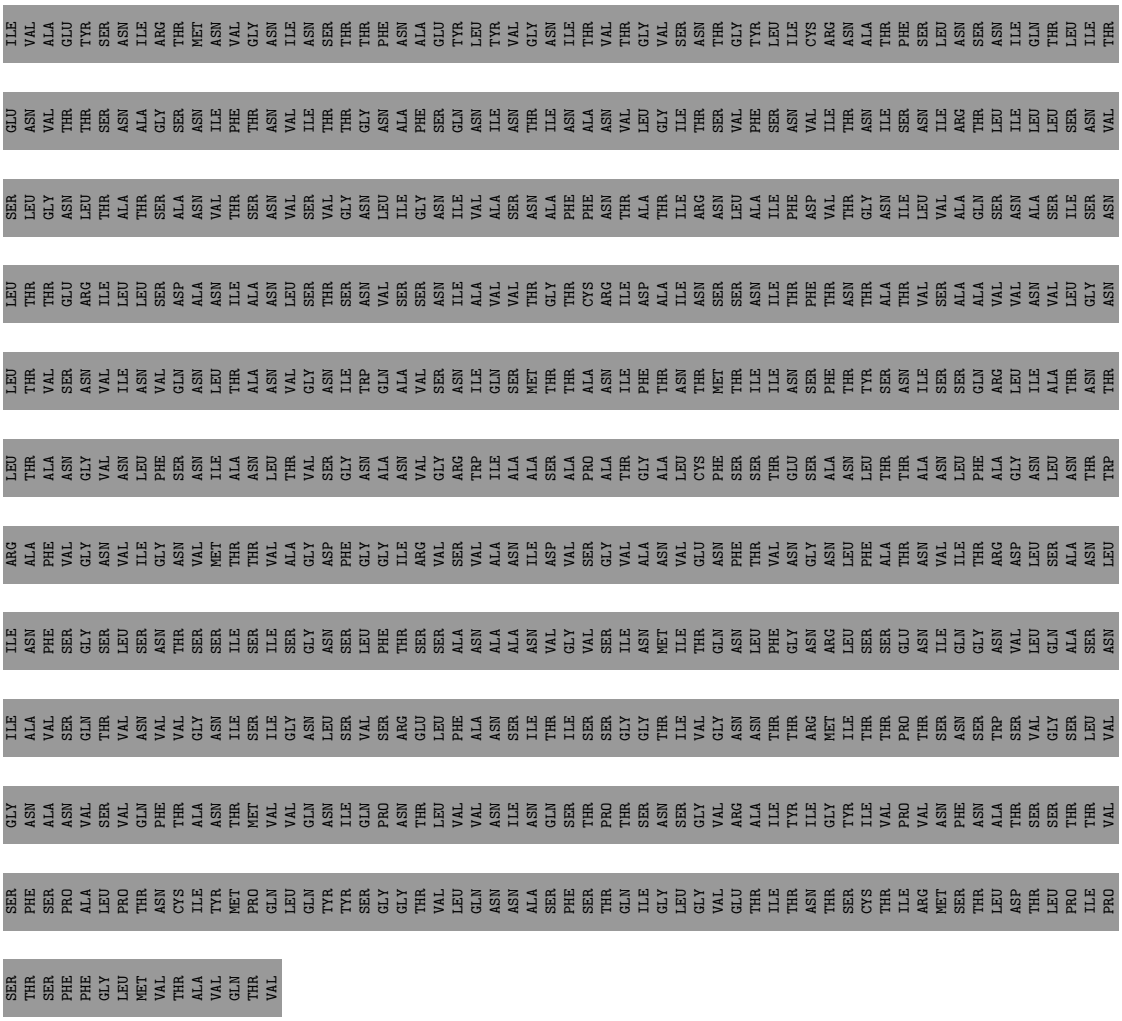

• Molecule 22: P20

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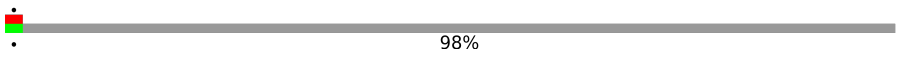
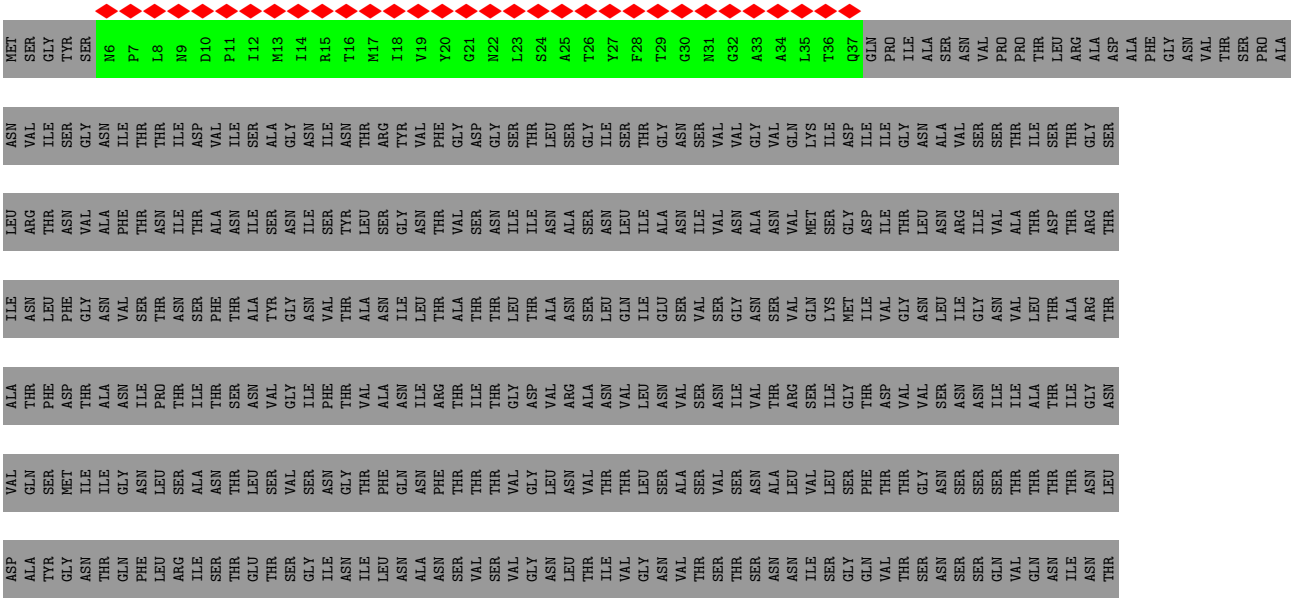
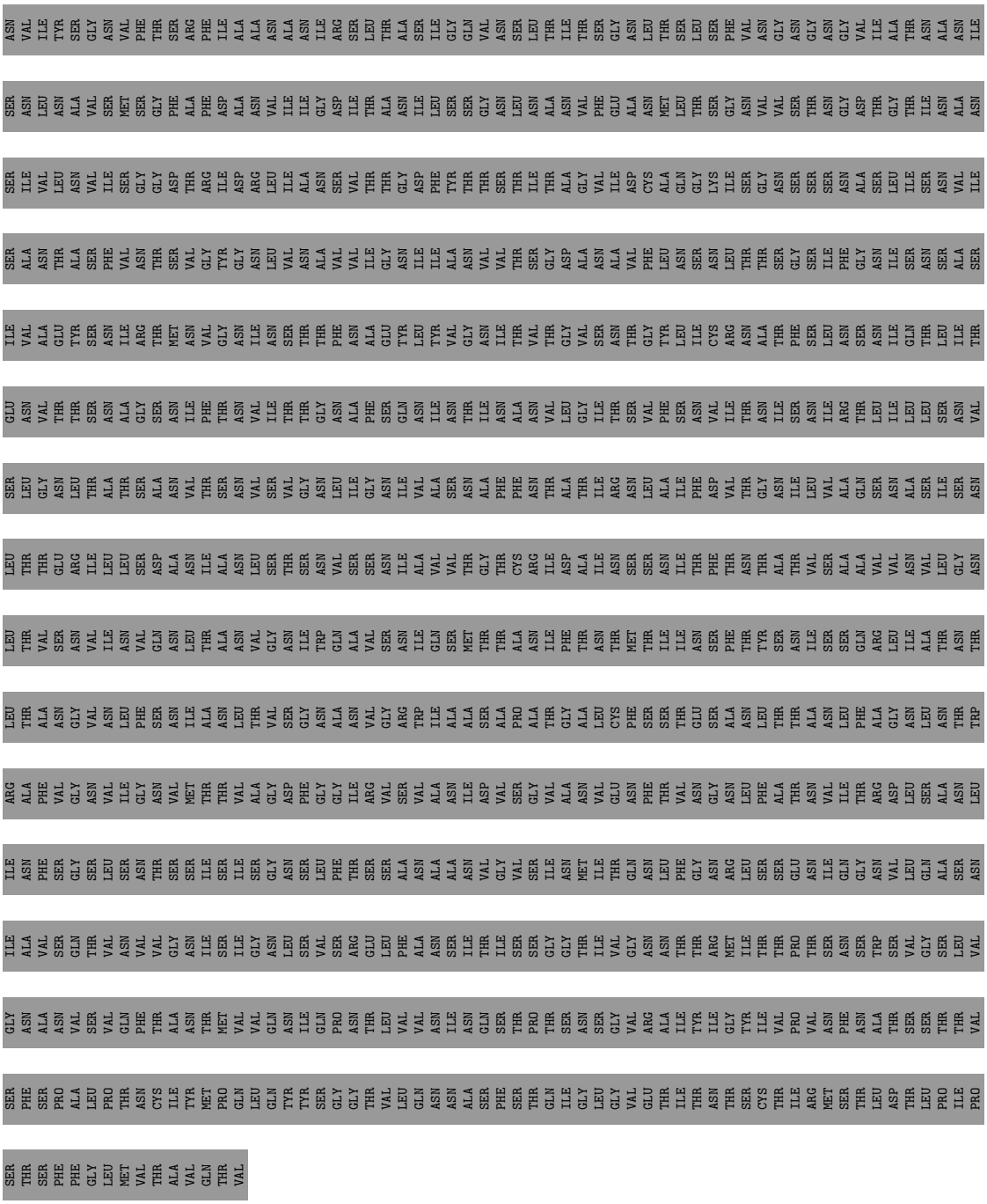
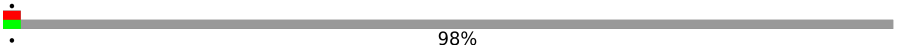


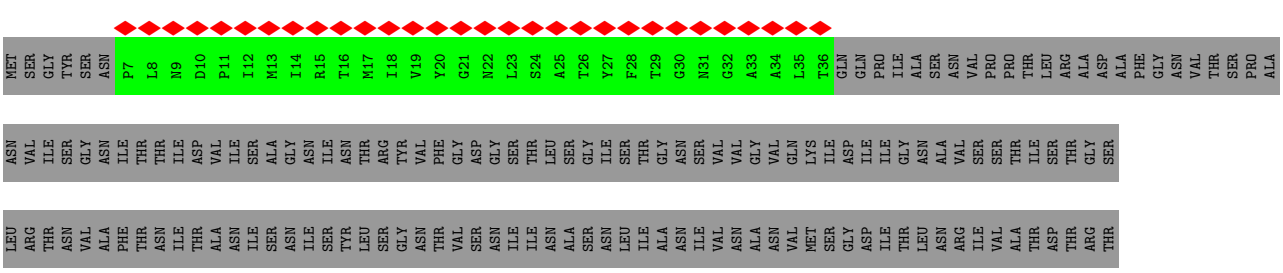


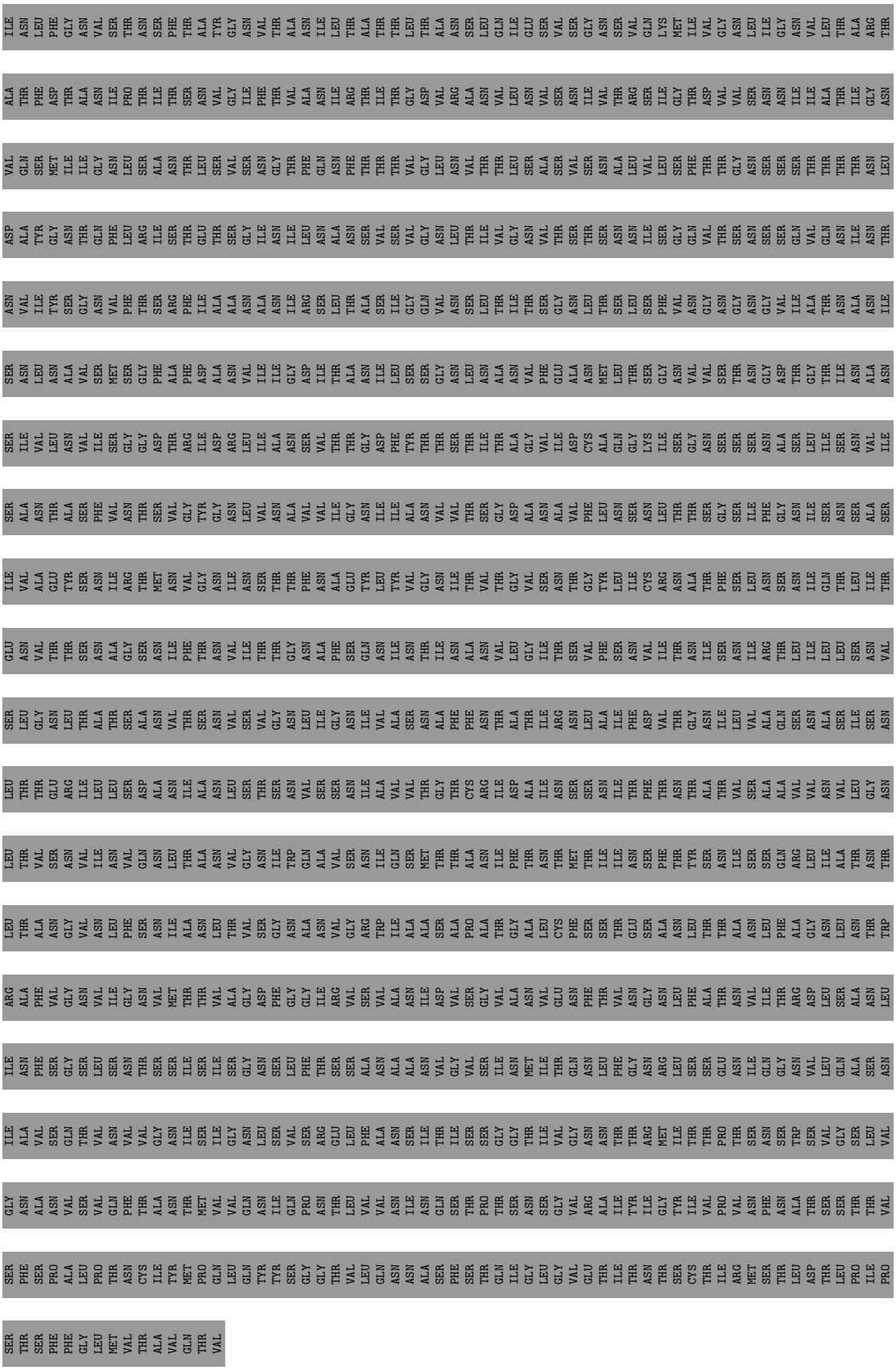


• Molecule 22: P20

Chain du:

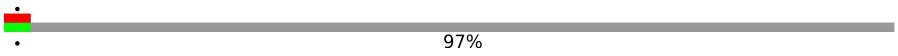






• Molecule 23: P21

Chain cP: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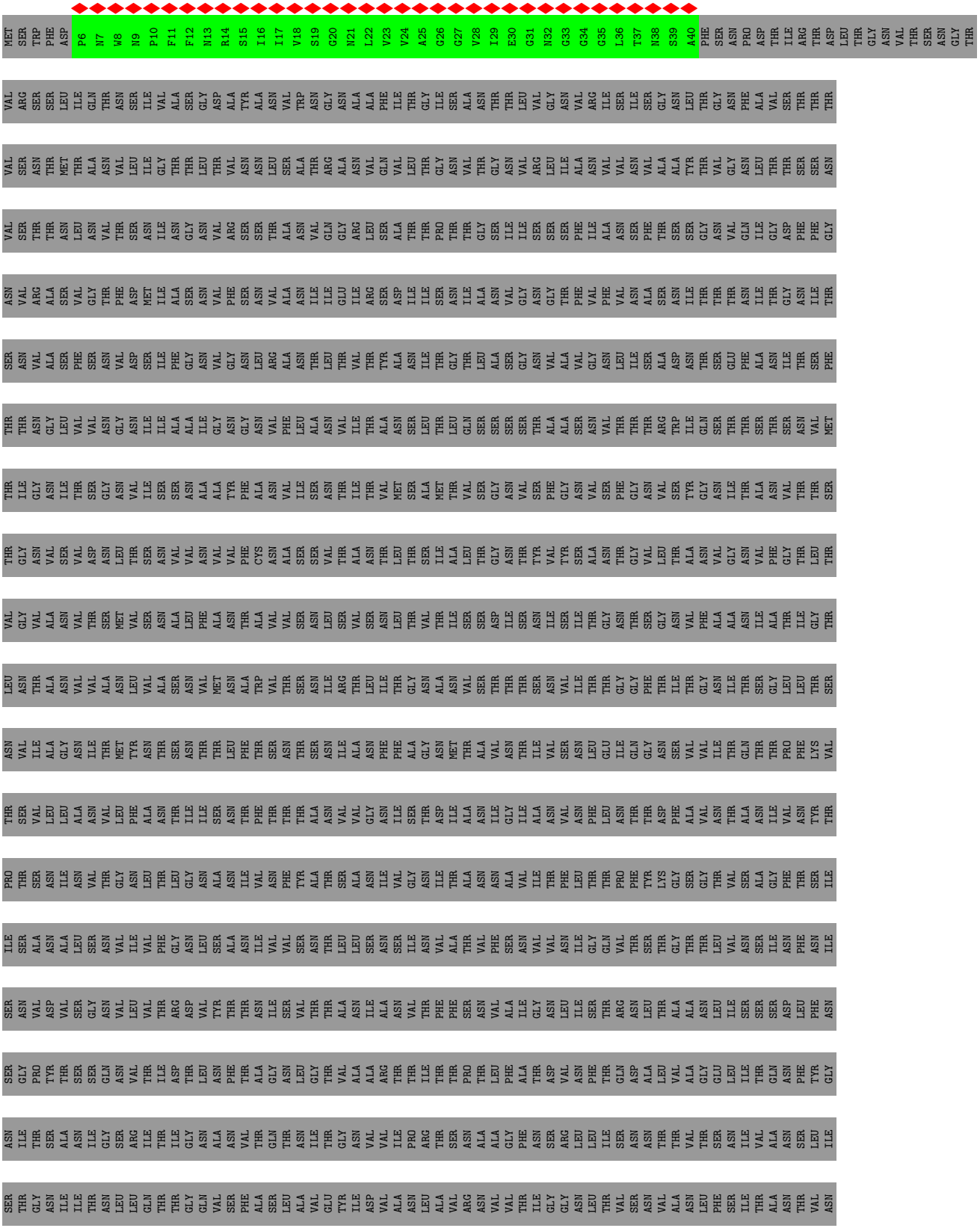
MET SER TRP PHE ASP P6 N7 W8 N9 P10 F11 F12 N13 R14 S15 I16 I17 V18 S19 G20 N21 L22 V23 V24 A25 G26 G27 V28 I29 E30 G31 N32 G33 G34 G35 L36 T37 N38 S39 A40 PHE SER ASN PRO ASP THR ILE ARG THR ASP LEU THR GLY ASN VAL THR SER ASN GLY THR
VAL ARG SER SER LEU ILE GLN THR ASN SER ILE VAL ALA SER GLY ASP ALA TYR ALA ASN VAL TRP ASN GLY ASN ALA ALA PHE ILE THR GLY ILE SER ALA ASN THR THR LEU VAL ALA GLY ASN PHE ALA VAL SER THR THR
VAL SER ASN THR MET THR ALA ASN VAL LEU ILE GLY THR THR VAL ASN ASN LEU SER ALA THR ARG ALA ASN VAL GLN VAL LEU THR GLY ASN VAL THR VAL LEU THR PRO THR THR GLY SER ASN THR GLY ASN VAL ARG LEU ILE ALA ASN VAL VAL ASN VAL ALA ALA TYR THR VAL GLY ASN LEU THR THR SER
VAL SER THR THR ASN LEU ASN VAL THR SER ASN ILE ASN GLY ASN VAL GLN GLY ARG LEU SER ALA THR THR PRO THR THR GLY SER ILE ILE SER SER PHE ILE ALA ASN SER PHE THR SER GLY ASN GLN ILE GLY ASP PHE PHE GLY
ASN VAL ARG ALA SER VAL GLY THR PHE ASP MET ILE ALA SER ASN VAL PHE SER ASN VAL ALA ASN ILE ILE ILE GLU ILE ARG SER ASP ILE ILE SER ASN ILE ILE THR PHE VAL PHE VAL ASN ALA SER ASN ILE THR THR THR ASN ILE THR THR
SER ASN VAL ALA SER PHE SER ASN VAL ASP ASN SER ILE PHE SER ASN VAL THR TYR ALA ASN ILE THR LEU THR VAL THR TYR ALA ASN ILE THR GLY ASN VAL ALA VAL GLY ASN LEU ILE SER ALA ASP ASN THR SER GLU PHE ALA ASN ILE THR SER PHE
THR THR ASN GLY LEU VAL VAL ASN GLY ASN ILE ILE ALA ALA ILE GLY ASN GLY ASN VAL LEU ILE THR ALA ASN VAL LEU THR LEU GLN SER SER SER SER THR ALA ALA SER ASN VAL THR THR THR ARG TRP ILE GLN SER THR THR SER THR SER ASN VAL MET
THR ILE GLY ASN ILE THR SER GLY ASN VAL ILE SER SER ASN ALA ALA ILE GLY ASN VAL PHE ALA ASN VAL ILE SER ASN THR ILE THR VAL MET SER ALA MET THR VAL SER GLY ASN VAL SER PHE GLY ASN VAL ASN VAL SER TYR GLY ASN ILE THR ALA ASN VAL THR THR SER
THR GLY ASN VAL SER VAL ASP ASN LEU THR SER ASN VAL VAL PHE CYS ASN ALA SER SER VAL THR ALA ASN THR LEU THR SER ILE ALA LEU THR GLY ASN THR TYR VAL TYR SER ALA ASN THR GLY VAL LEU THR ALA ASN VAL GLY ASN VAL PHE GLY THR LEU THR
VAL GLY VAL ALA ASN VAL THR SER MET VAL SER ASN ALA LEU PHE ALA ASN THR ALA VAL VAL SER ASN LEU SER VAL SER ASN LEU THR SER VAL THR ILE SER SER ASP ILE SER ASN ILE SER ILE THR GLY ASN THR SER GLY ASN VAL PHE ALA ALA ASN ILE ILE GLY THR
LEU ASN THR ALA ASN VAL VAL ALA ASN LEU VAL VAL ALA SER ASN VAL MET ASN ALA TRP VAL VAL THR SER ASN ILE ARG THR LEU ILE THR ILE GLY ASN ALA ASN VAL SER THR THR THR SER ASN VAL ILE THR THR GLY GLY PHE THR ILE THR ILE THR SER GLY LEU LEU THR SER
ASN VAL ILE ALA ASN GLY ASN ILE THR MET TYR ASN THR SER ASN THR THR LEU PHE THR SER ASN THR SER ASN ILE ALA ASN PHE PHE ALA GLY ASN MET THR ALA VAL ASN ILE ILE SER ASN THR ILE VAL SER ASN VAL LEU GLU ILE GLN GLY ASN SER VAL VAL ILE THR GLN THR THR PRO PHE LYS VAL
THR SER VAL LEU LEU ALA ASN VAL LEU PHE ALA ASN THR ILE ILE SER ALA ASN VAL ALA ASN VAL VAL GLY ASN ILE SER THR ASP ILE ALA ASN ILE GLY ILE ILE ALA ASN VAL ASN PHE LEU ASN THR THR ASP PHE ALA VAL ASN THR ALA ASN ILE ILE VAL SER
PRO THR SER ASN ILE ASN VAL THR GLY ASN LEU THR LEU GLY ASN ALA ASN PHE TYR ALA THR SER ALA ASN ILE VAL GLY ASN ILE THR ALA ASN ASN ASN ALA VAL ILE THR PHE LEU THR THR PRO THR PHE TYR LYS GLY SER GLY THR VAL THR SER
ILE SER ALA ASN ASN VAL THR LEU LEU SER ASN SER ILE ASN VAL ALA PHE SER ASN VAL ASN ILE GLY GLN VAL THR SER THR GLY THR ILE ASN GLY LEU THR ALA ASN ASN ILE ILE SER
SER ASN VAL ASP VAL SER VAL LEU VAL THR THR ILE ARG ASP VAL TYR THR THR ASN ILE SER VAL THR THR ALA ASN ILE ILE GLY ASN LEU ILE SER THR ARG ASN LEU THR ALA ASN LEU ILE SER ASP LEU PHE ASN
SER GLY PRO TYR THR SER SER GLN ASN VAL THR ILE ASP THR LEU GLY ALA ALA ARG THR THR ILE THR THR PRO THR THR GLY SER ALA THR ASP VAL ASN PHE THR GLN THR ALA LEU VAL ALA ALA GLY GLU LEU ILE THR GLN ASN PHE TYR GLY
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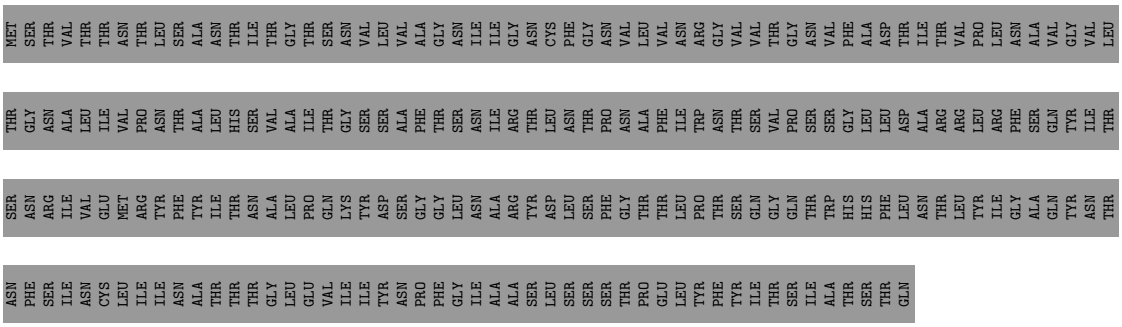
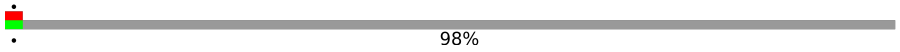
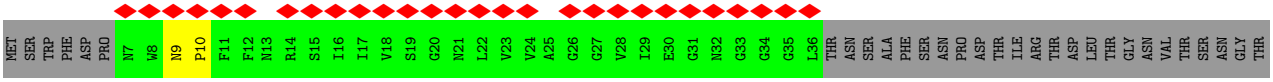
SER THR GLY ASN ILE ILE THR ASN LEU GLN THR THR GLY GLN VAL SER PHE ALA SER LEU ALA VAL GLU TYR ILE ASP VAL ALA ASN LEU ALA VAL ASN ASN VAL ALA ASN LEU THR VAL ILE GLY GLY ASN LEU THR VAL SER ASN VAL ALA ASN LEU ILE SER ILE THR ALA ASN ILE ASN

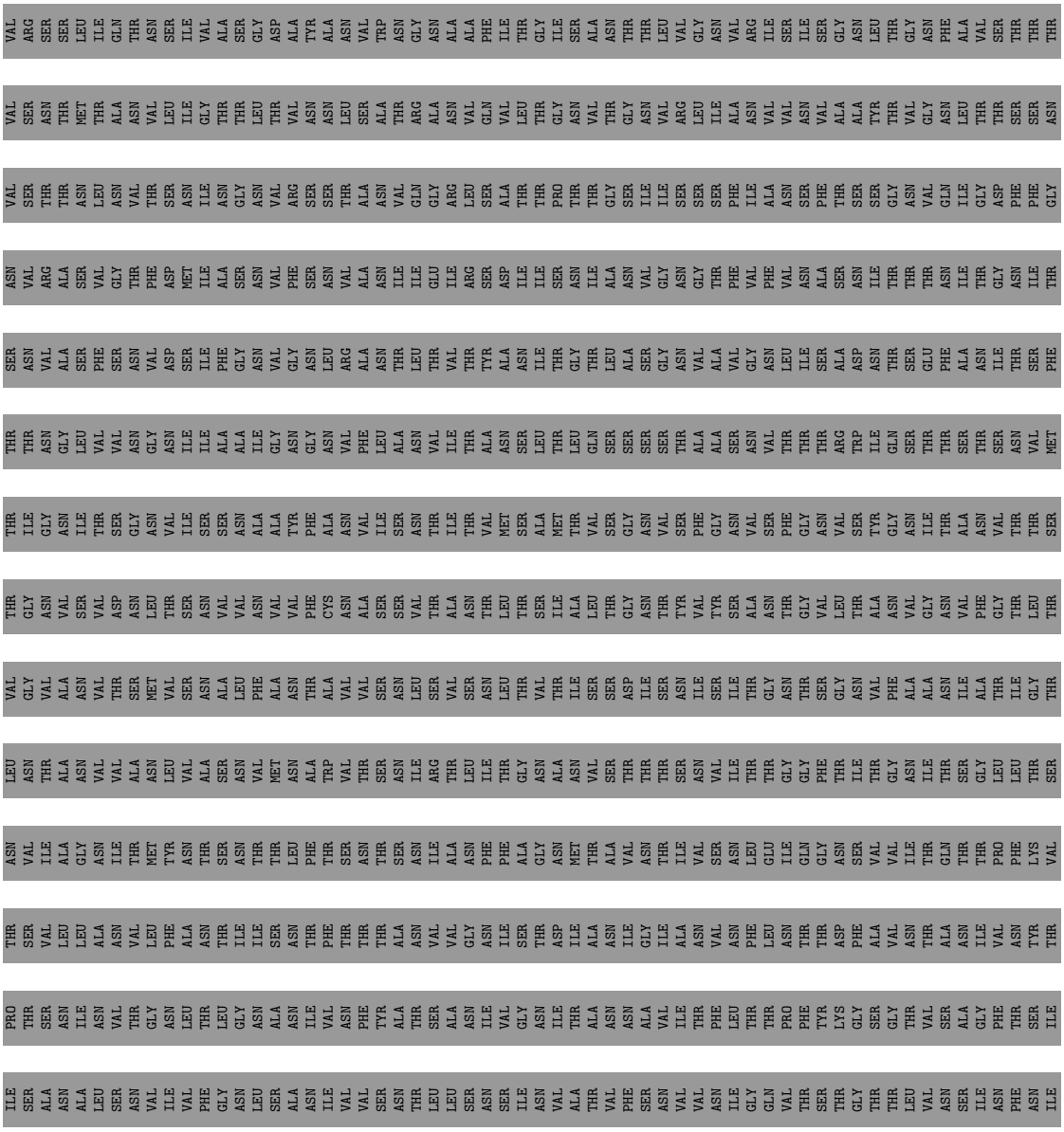


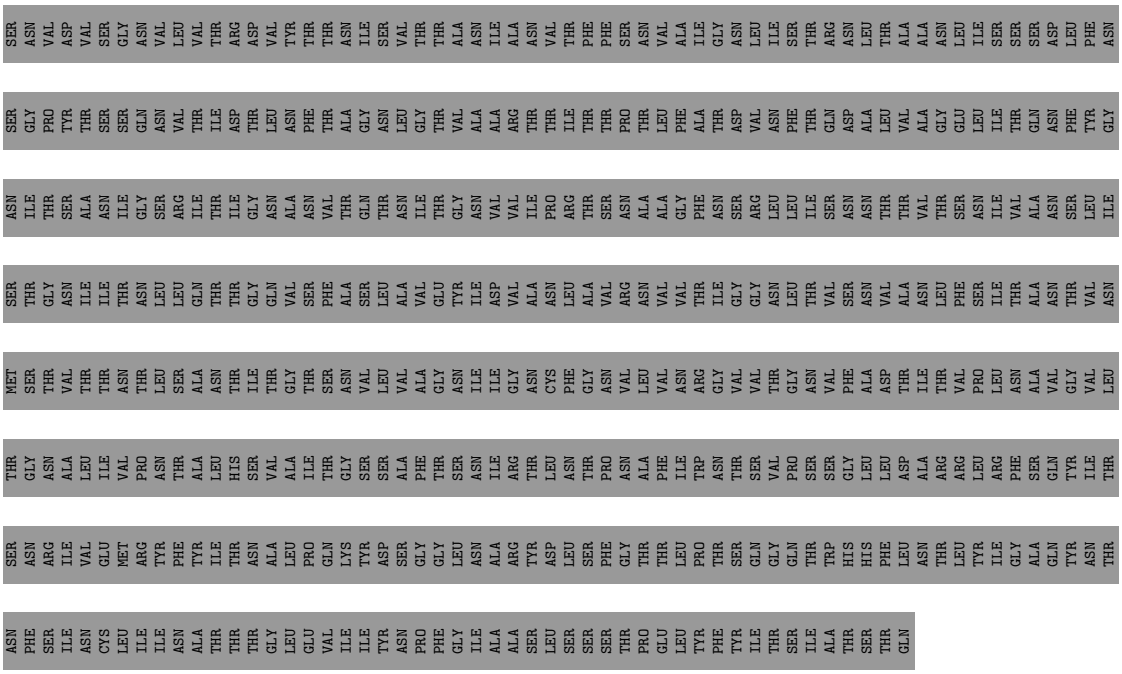
• Molecule 23: P21

Chain db:



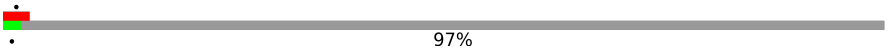


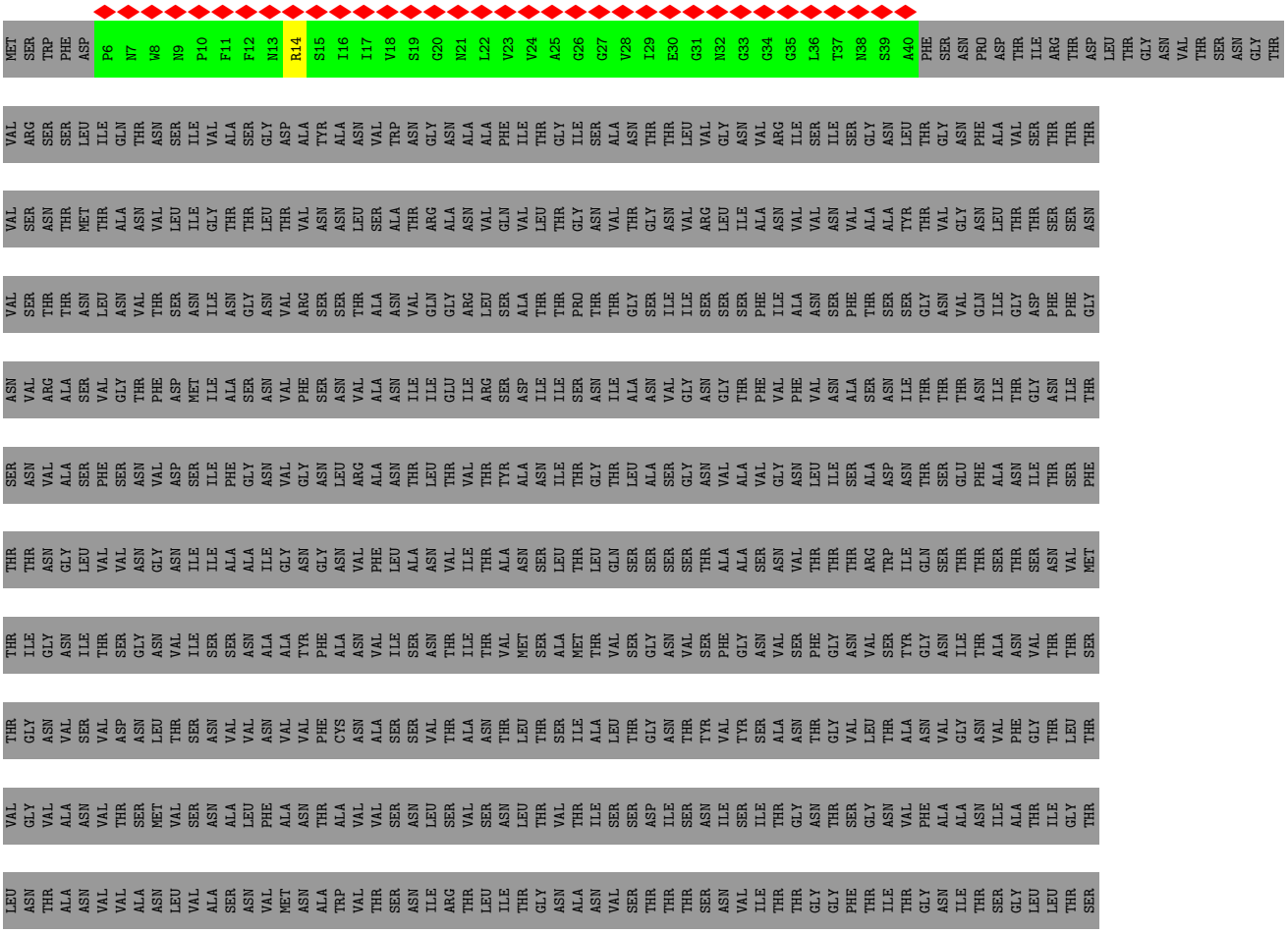


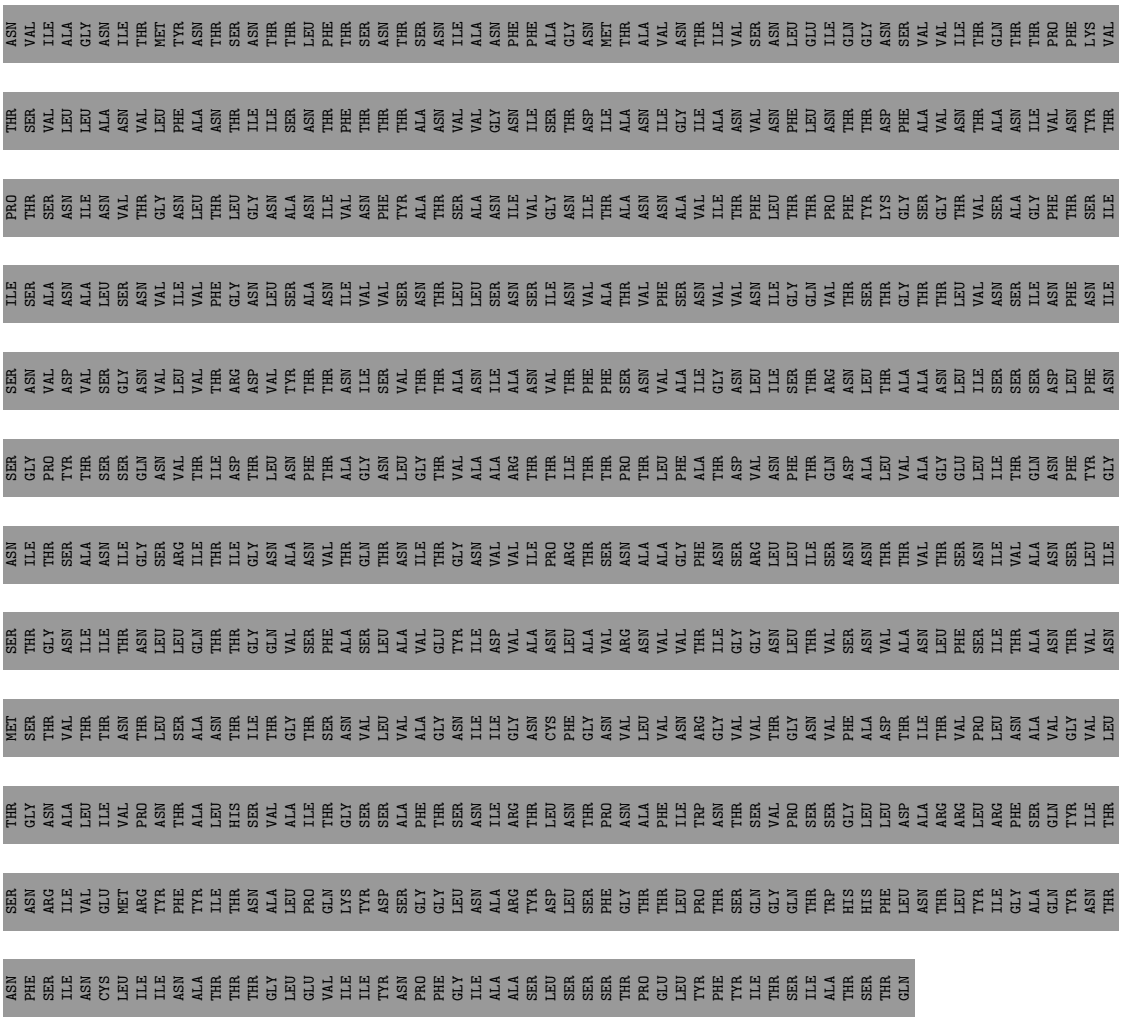


• Molecule 23: P21

Chain dh:

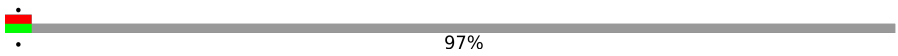


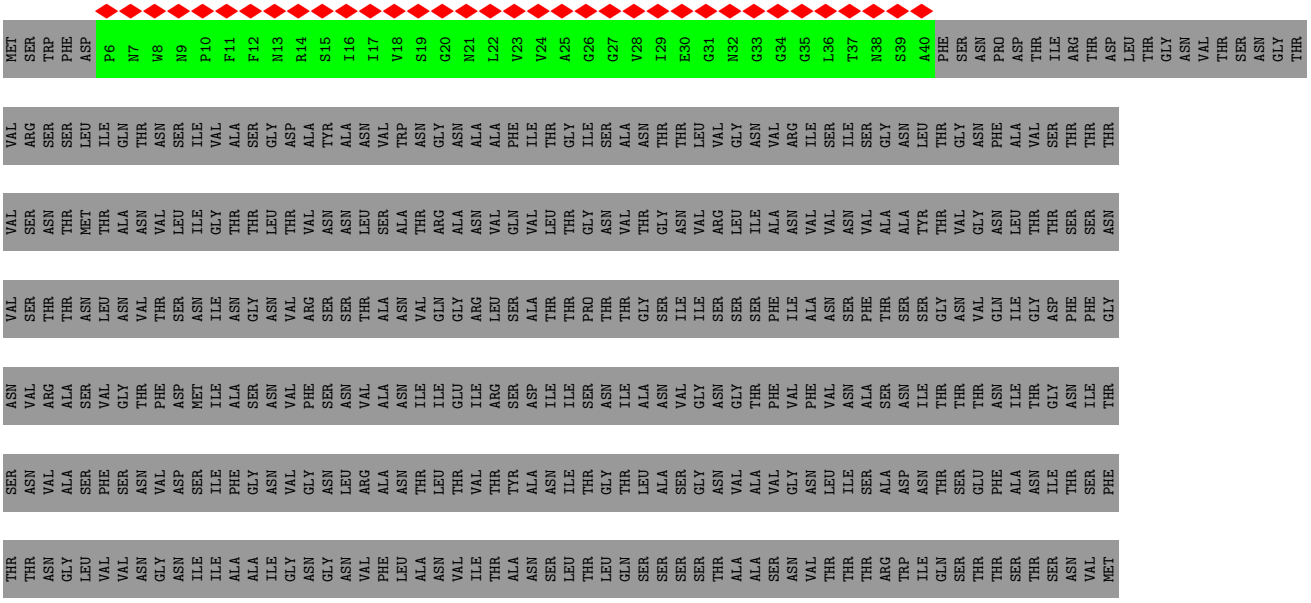


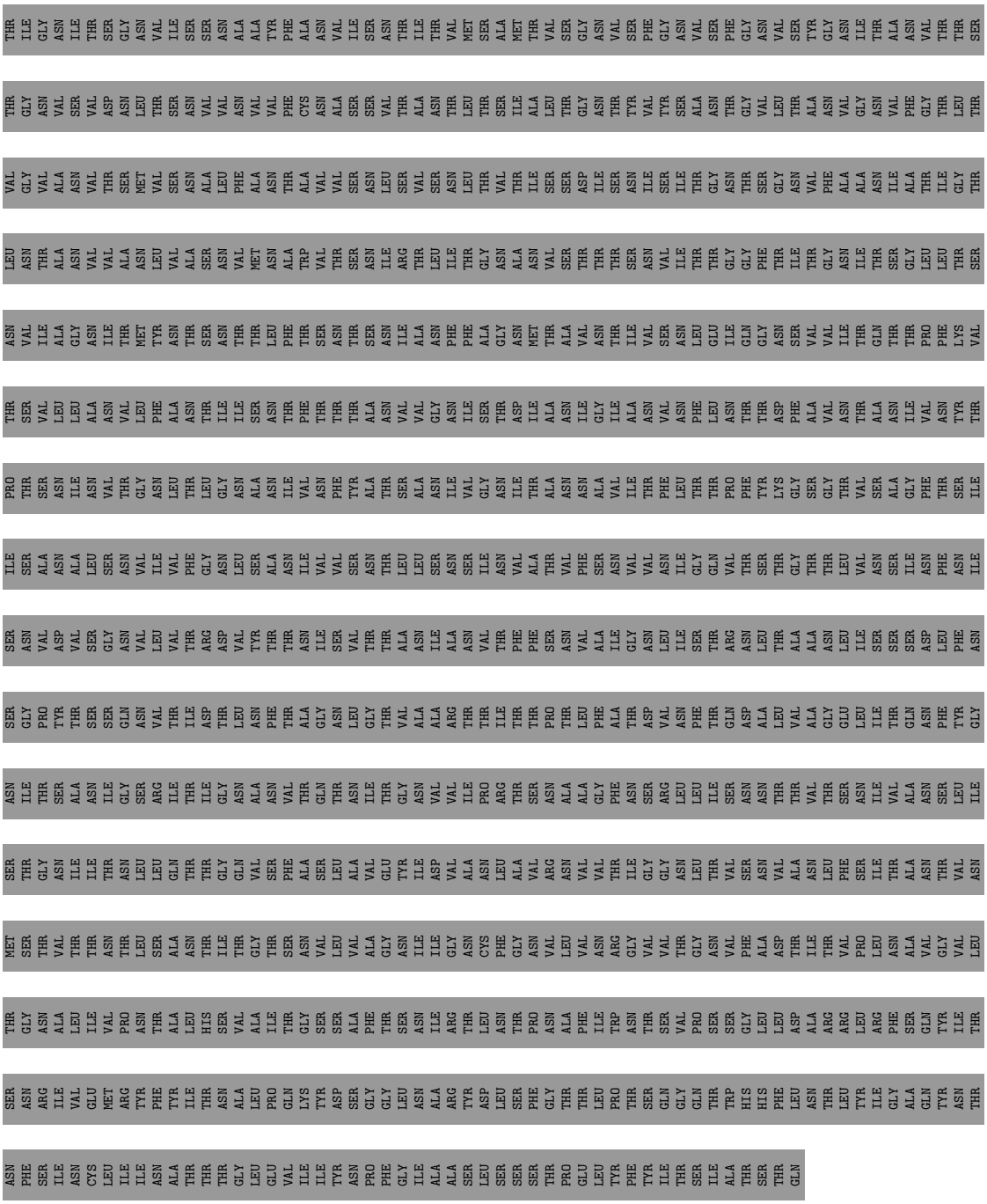


• Molecule 23: P21

Chain dt:

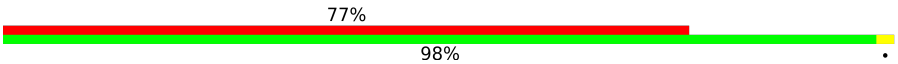


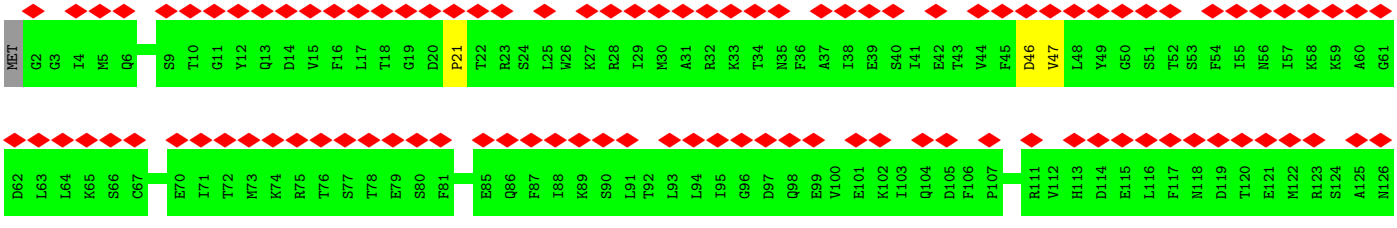


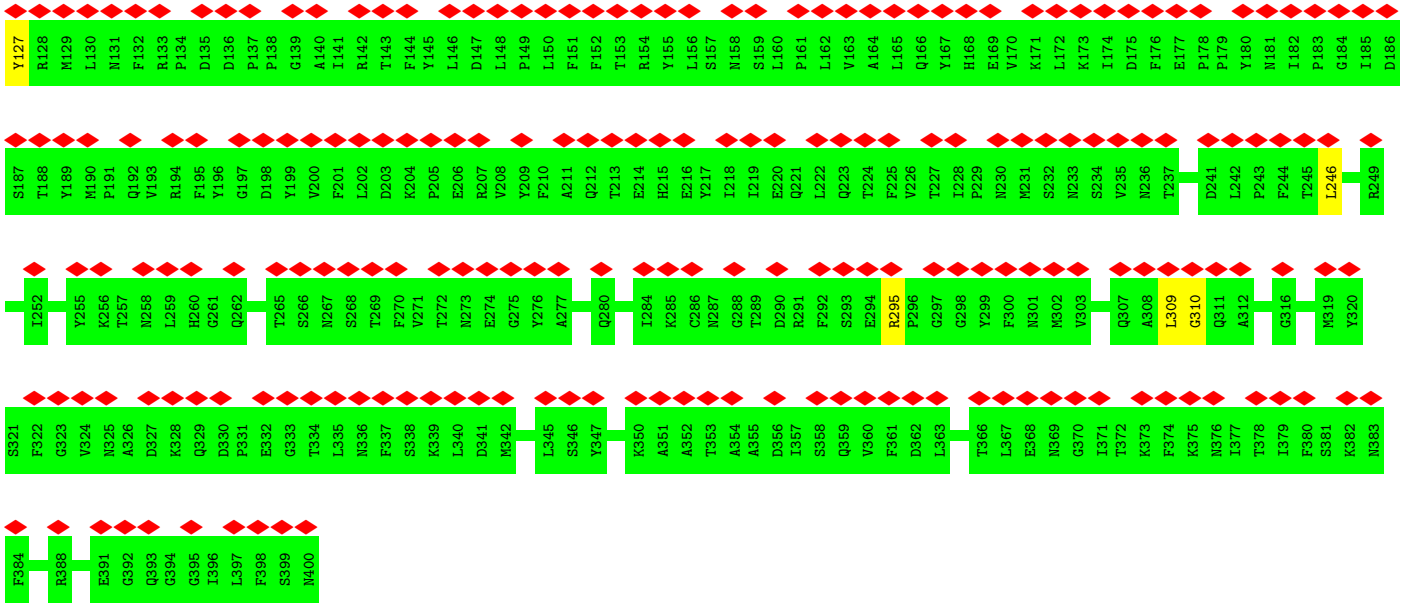


• Molecule 24: MCPv5

Chain cR:

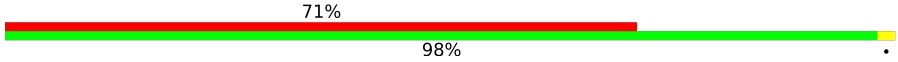


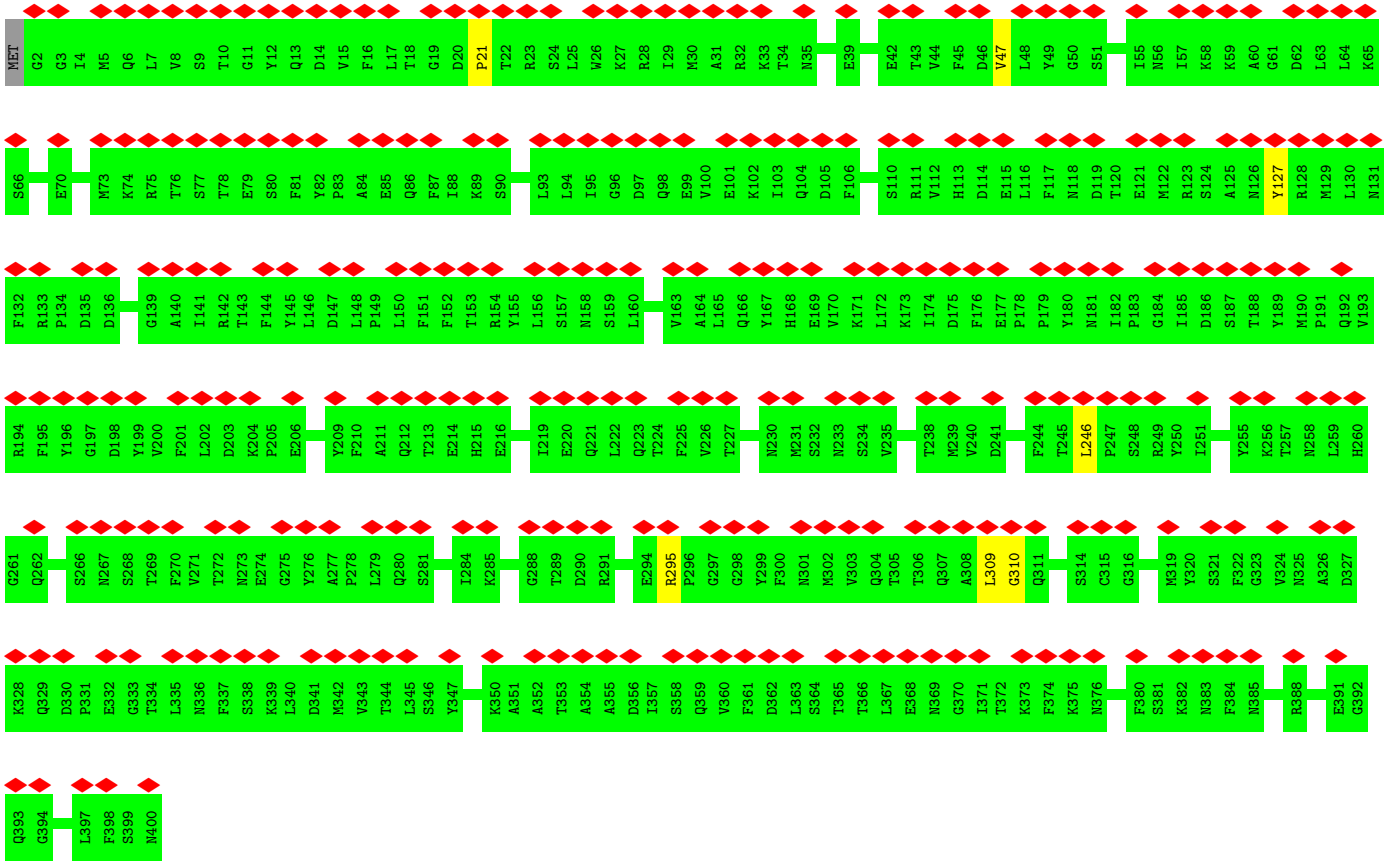




• Molecule 24: MCPv5

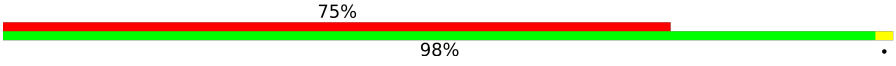
Chain cS:

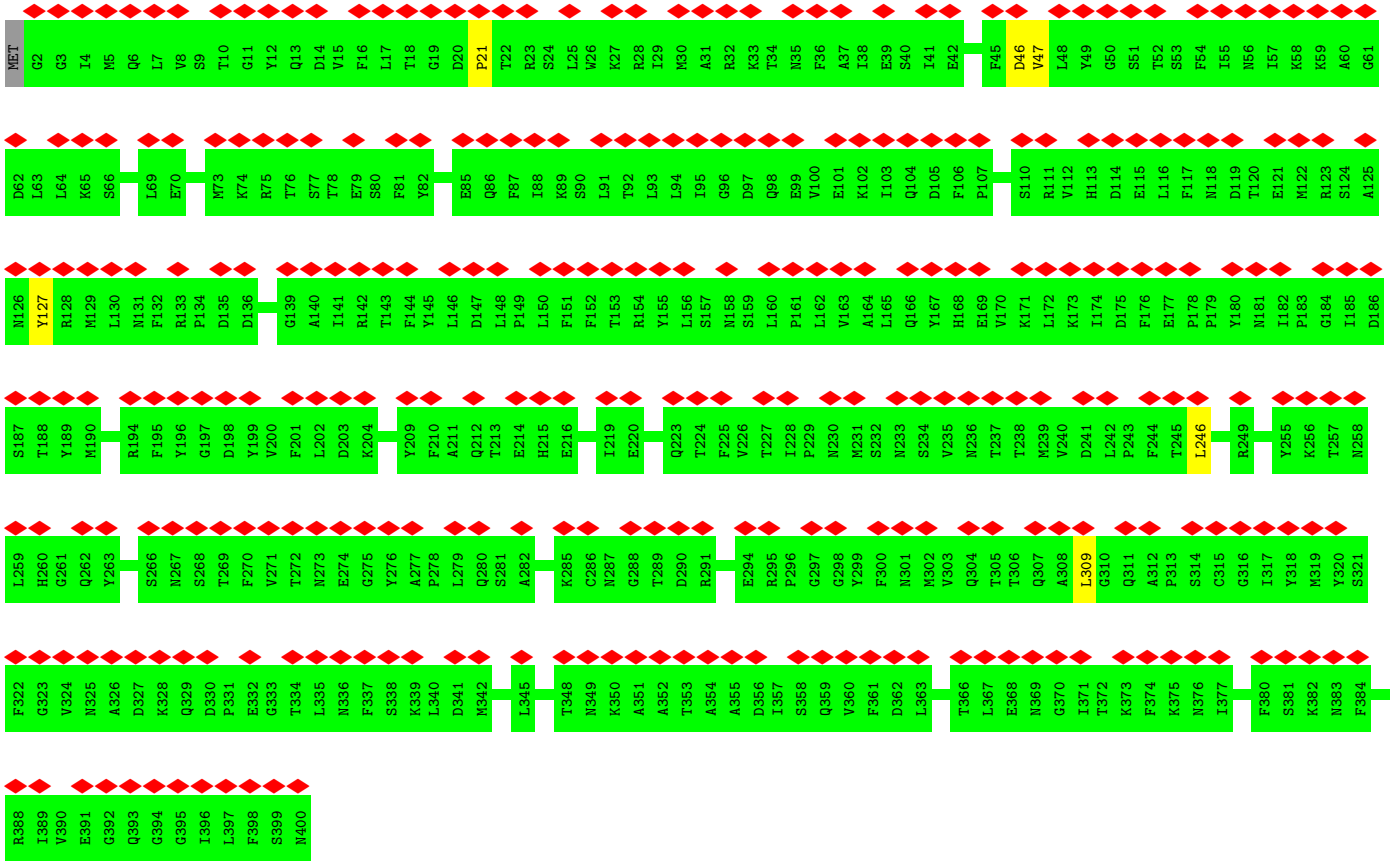




• Molecule 24: MCPv5

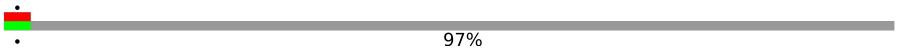
Chain cT:

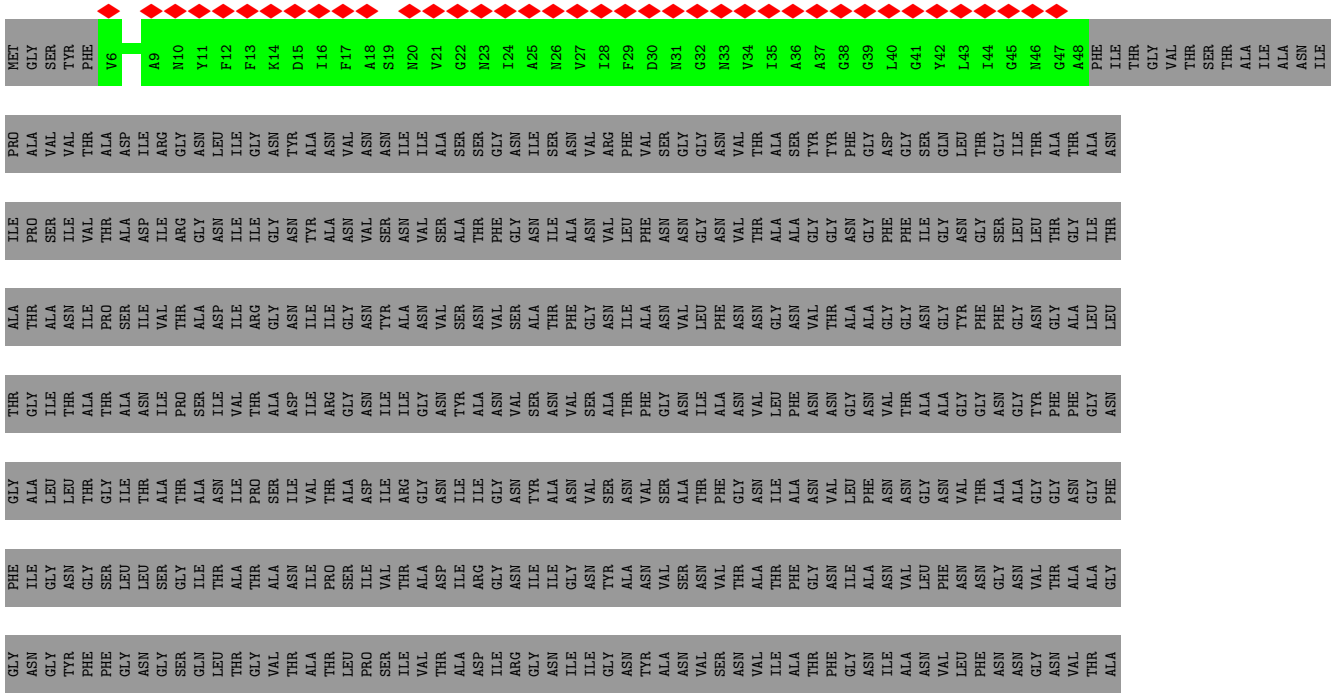


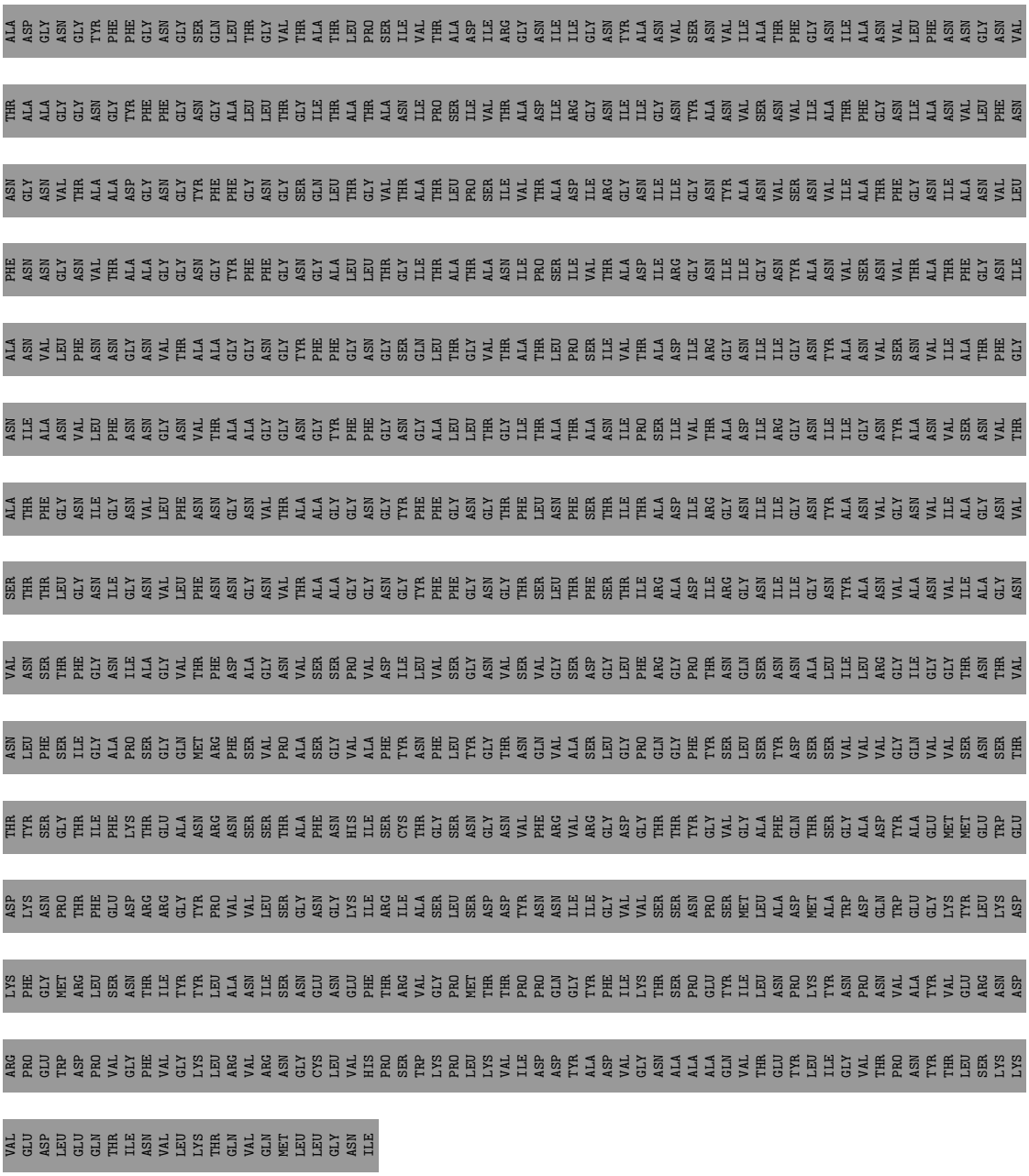


• Molecule 25: P22

Chain cU:

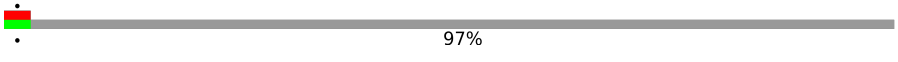


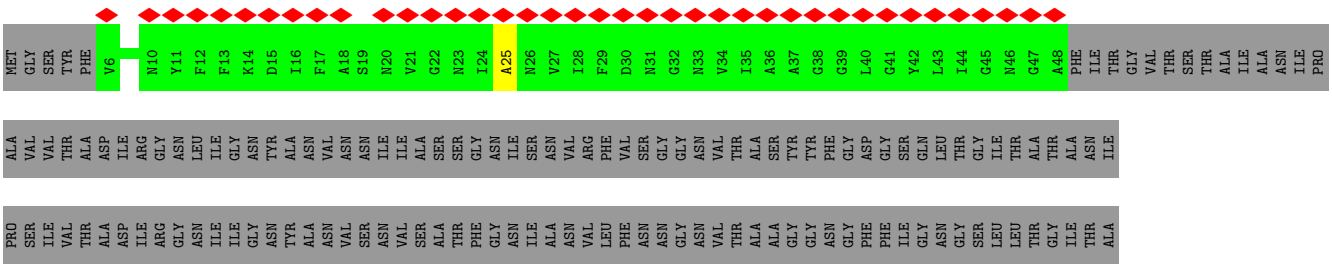


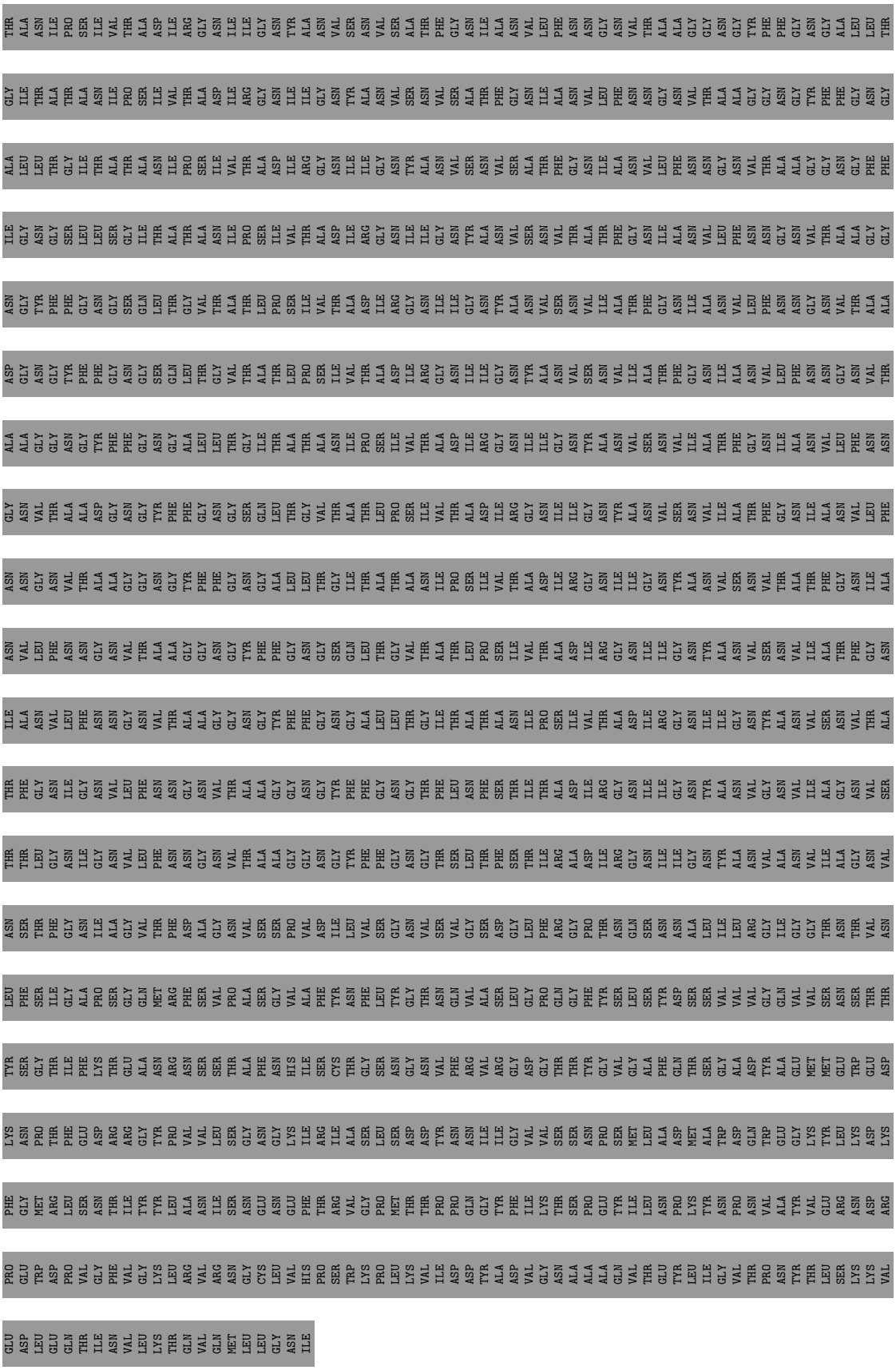


• Molecule 25: P22

Chain cV:






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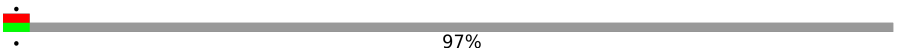
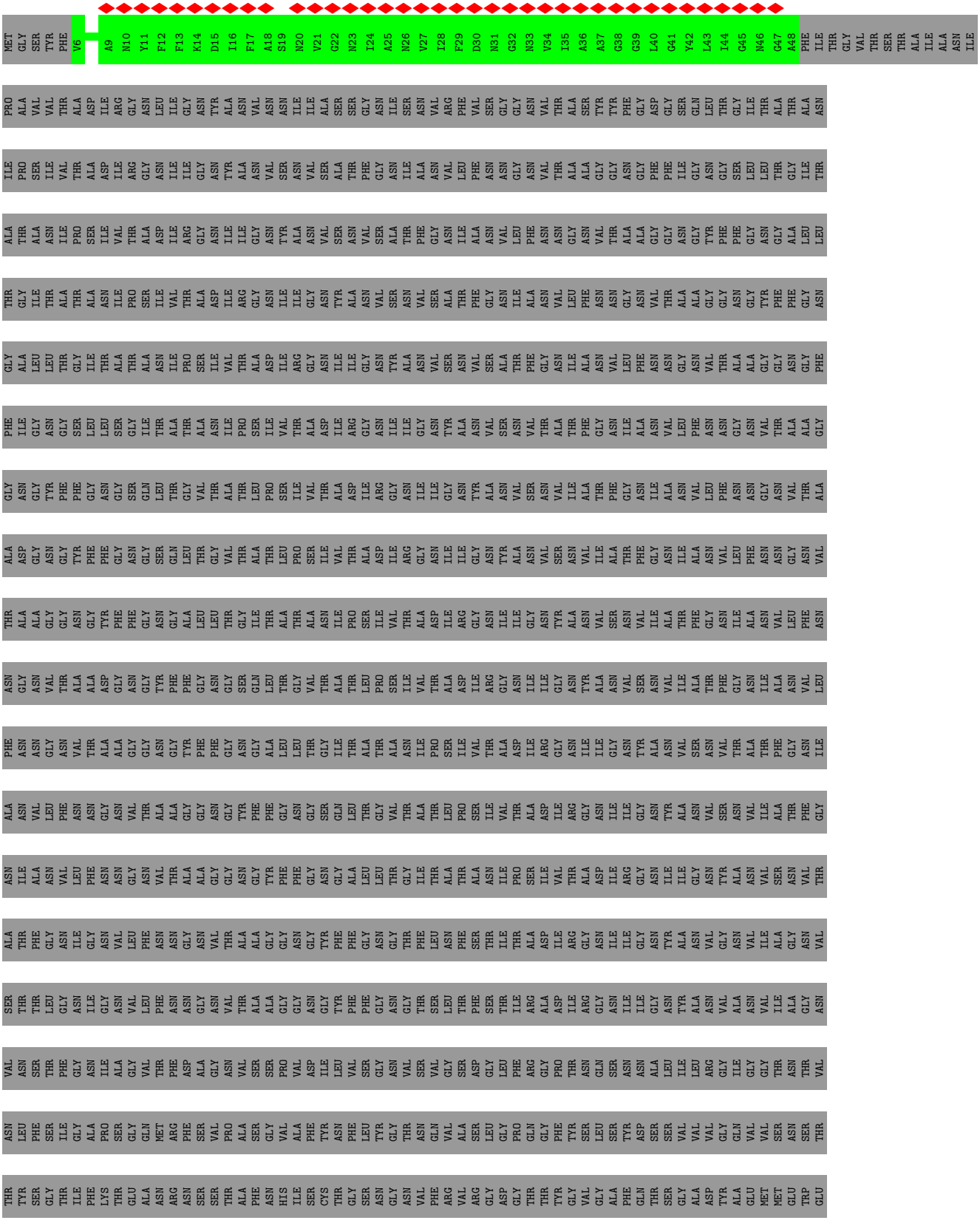
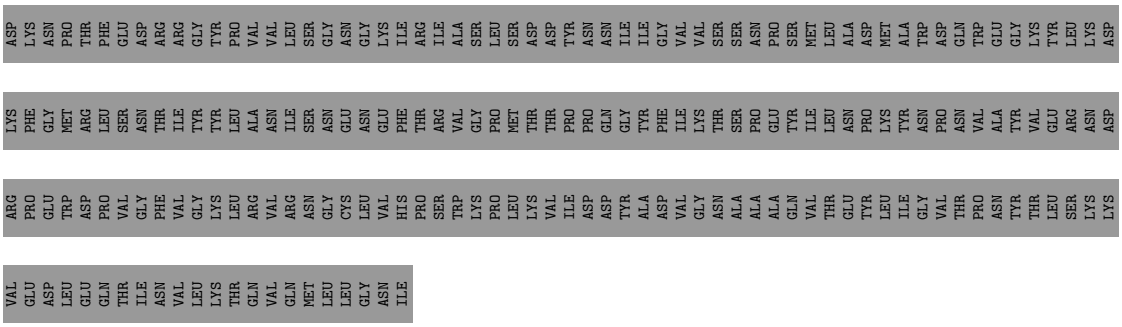
THR PHE GLY ASN ILE GLY ASN VAL LEU PHE ASN ASN GLY ASN VAL THR ALA ALA GLY GLY ASN GLY TYR PHE PHE GLY ASN GLY SER GLN LEU THR GLY VAL THR ALA THR LEU PRO SER ILE VAL THR ALA ASP ILE ARG GLY ASN ILE ILE GLY ASN TYR ALA ASN VAL SER ASN VAL ILE ALA THR PHE GLY ASN ILE ALA ASN VAL LEU PHE ASN ASN GLY ASN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

Chain cW:

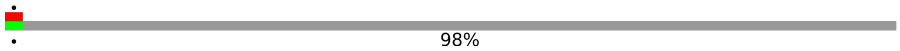


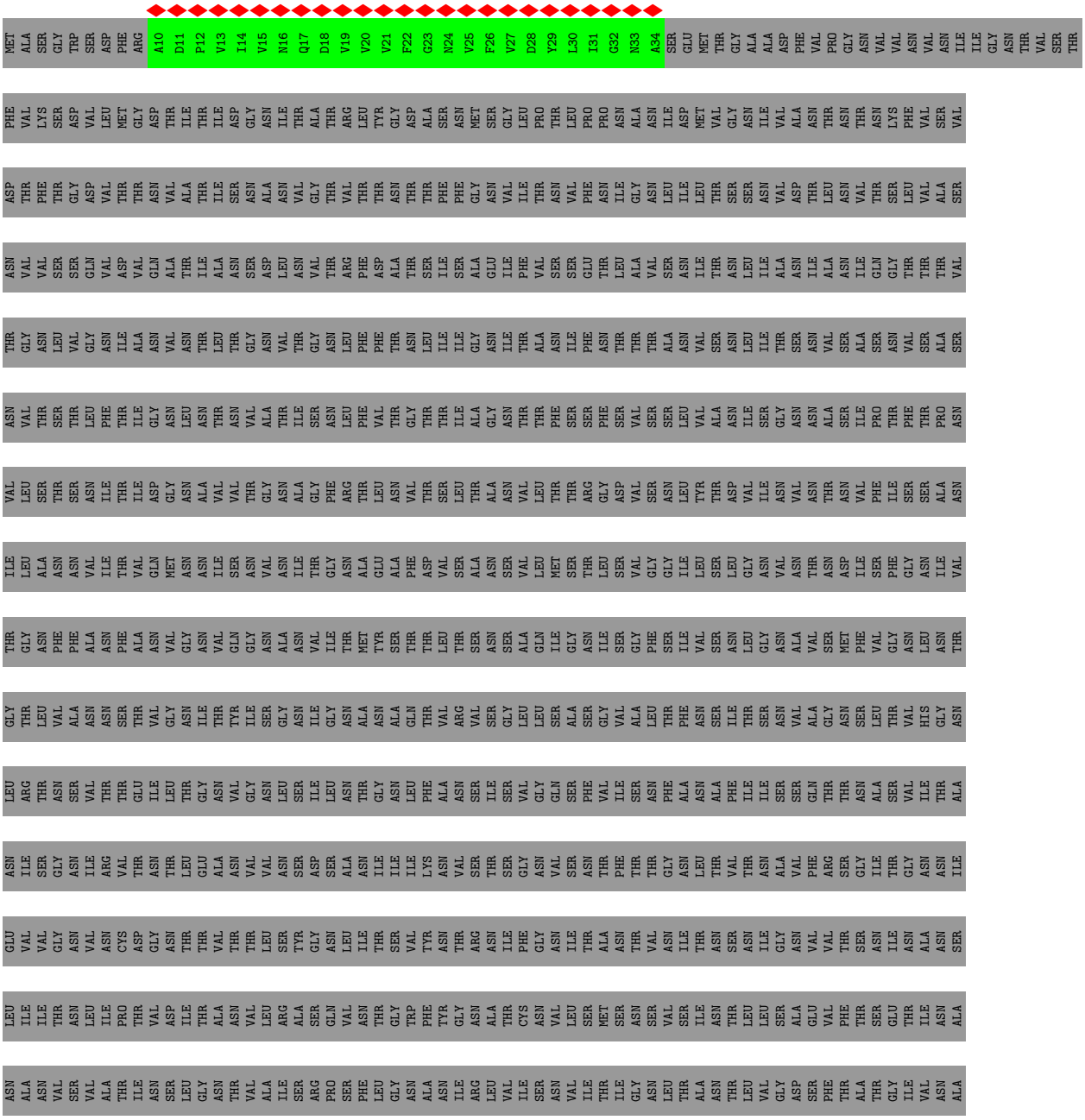


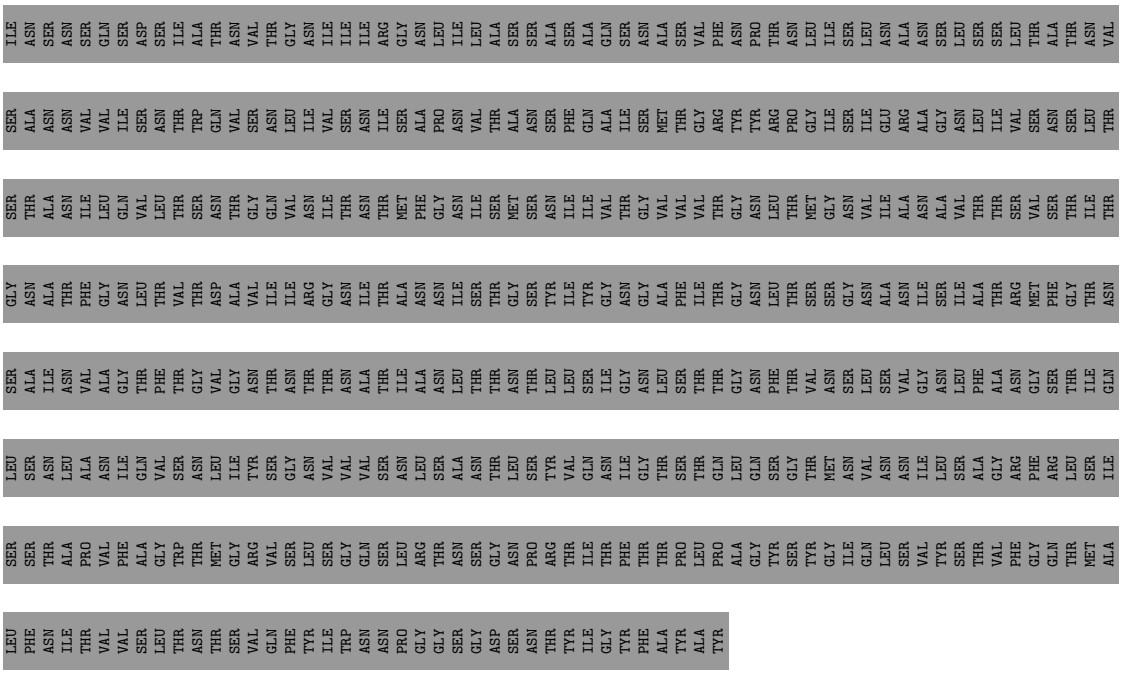


• Molecule 26: P23

Chain dm:

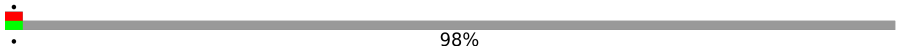


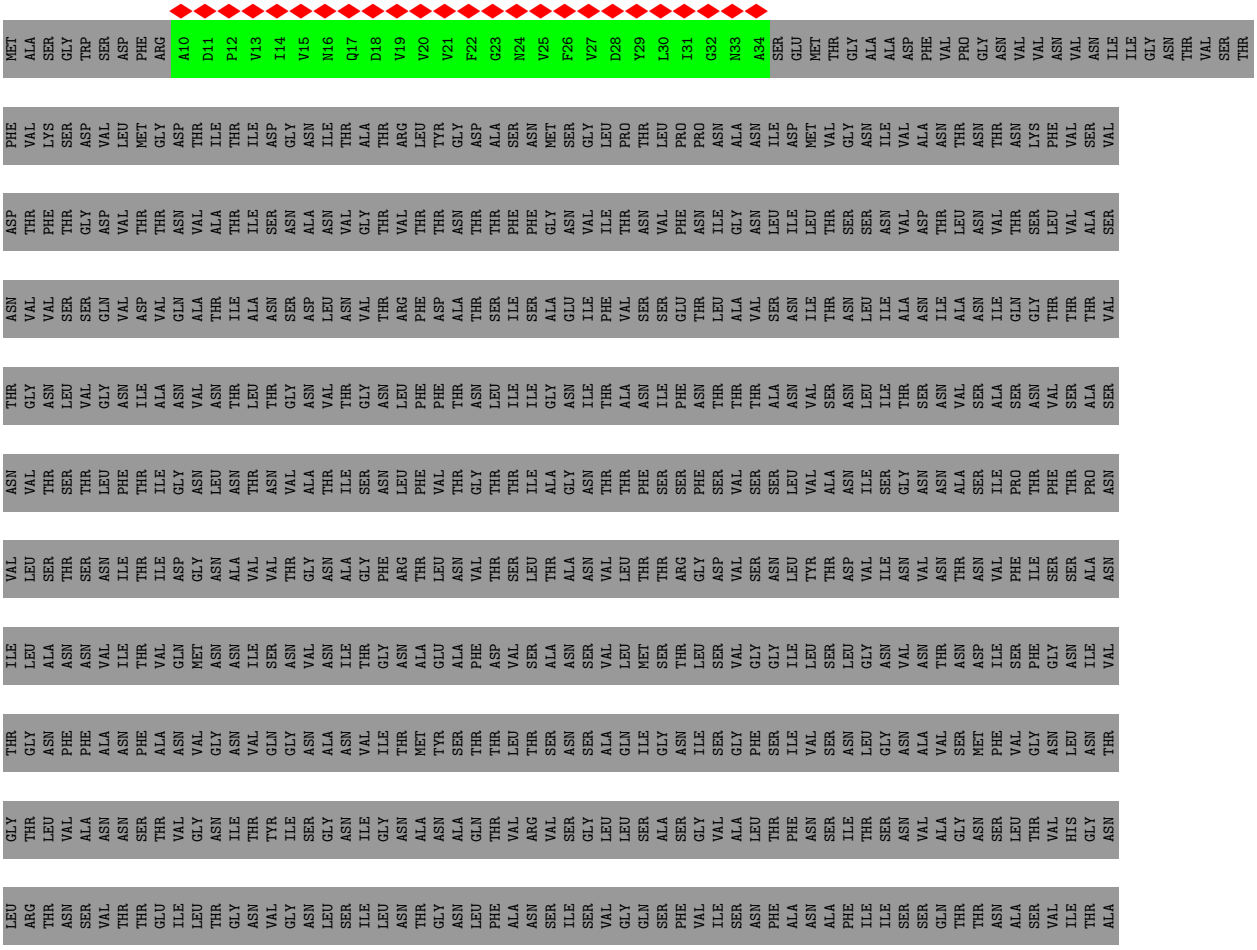


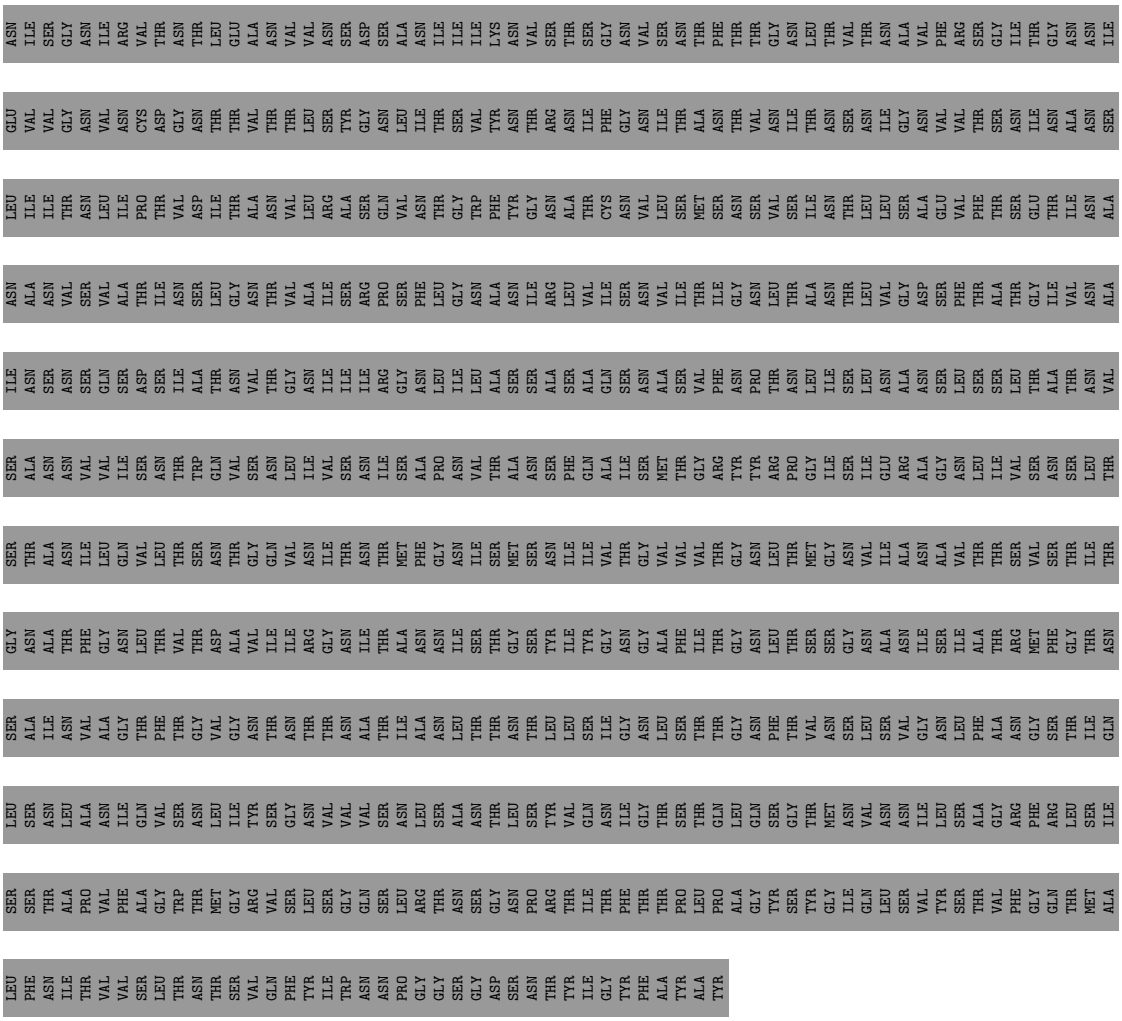


• Molecule 26: P23

Chain dn:

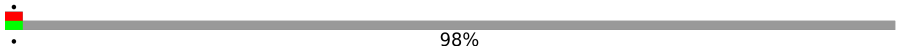


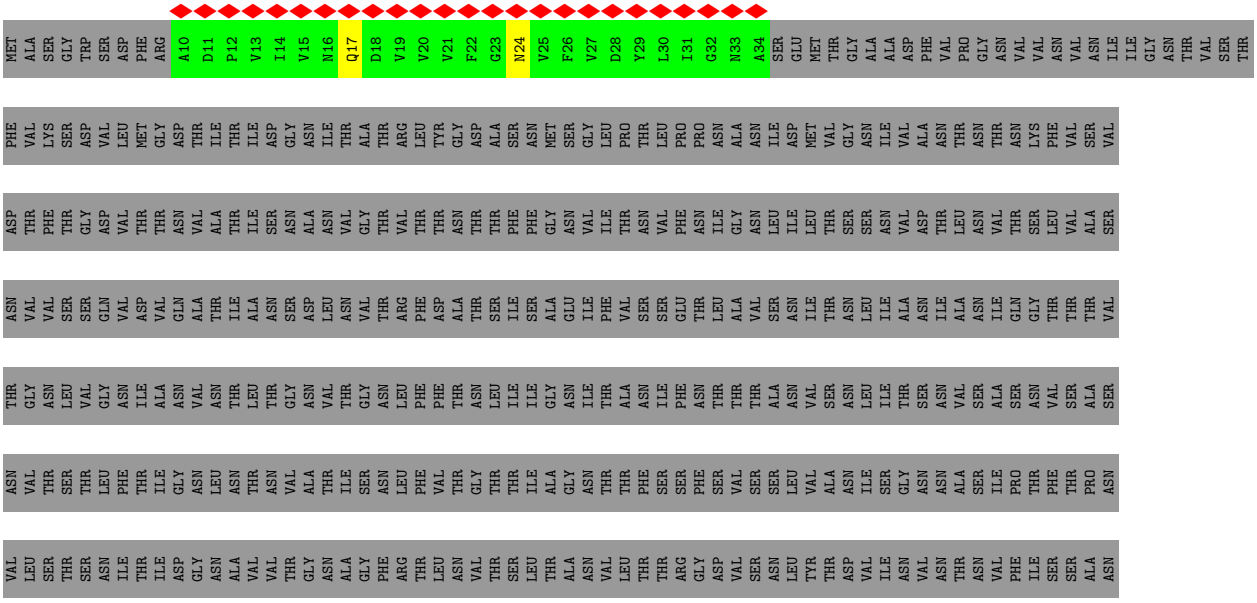


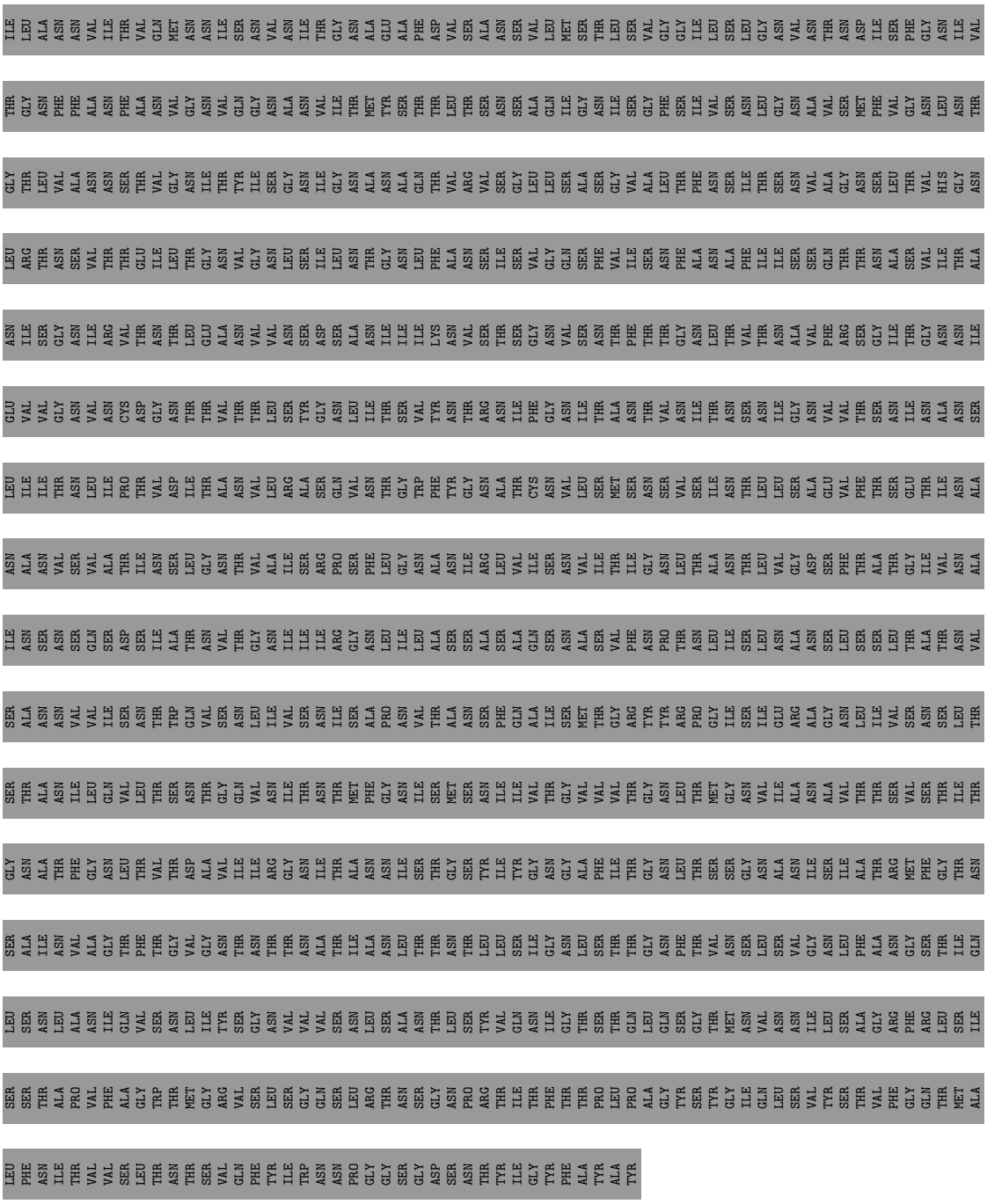


• Molecule 26: P23

Chain do:






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

4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	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.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
14	cd	172	ASN	C-N-CA	-5.61	107.69	121.70
24	cT	309	LEU	CA-CB-CG	5.42	127.77	115.30
14	cc	134	PRO	CA-N-CD	-5.41	103.92	111.50
24	cR	309	LEU	CA-CB-CG	5.38	127.66	115.30
1	ad	68	THR	N-CA-C	5.34	125.42	111.00
24	cS	309	LEU	CA-CB-CG	5.33	127.57	115.30
26	do	17	GLN	N-CA-C	5.25	125.18	111.00
5	cY	362	TYR	N-CA-C	5.12	124.83	111.00
5	dq	362	TYR	N-CA-C	5.12	124.83	111.00
5	de	362	TYR	N-CA-C	5.11	124.78	111.00
1	aK	4	GLY	C-N-CA	-5.05	109.08	121.70
1	ac	33	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

All (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
2	bA	382	ALA
6	bG	134	THR
7	bH	407	PRO
9	bO	21	LYS
11	bQ	79	PRO
14	cb	197	ASP
14	cc	167	GLY
15	cf	90	VAL
15	cf	126	SER
16	cg	82	CYS

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Mol	Chain	Res	Type
16	cg	88	GLN
21	ct	306	CYS
21	cF	70	ASN
1	al	123	ASN
1	as	123	ASN
1	at	123	ASN
1	aw	323	GLN
1	aI	123	ASN
1	aK	123	ASN
1	aO	123	ASN
1	aR	123	ASN
1	aT	123	ASN
1	aV	123	ASN
1	bg	123	ASN
1	bh	123	ASN
1	bj	123	ASN
1	bn	123	ASN
1	bp	123	ASN
2	bv	89	ALA
2	bx	89	ALA
2	by	89	ALA
2	bB	143	SER
13	bS	28	PRO
13	bS	31	ASP
14	bY	138	ALA
17	ch	72	SER
18	ci	36	PRO
21	cq	128	PHE
21	cF	98	PRO
21	cL	264	PRO
24	cR	310	GLY
24	cS	310	GLY
4	cX	273	PHE
5	cY	358	VAL
4	df	272	PRO
4	dk	273	PHE
4	dr	272	PRO
1	aH	123	ASN
1	aK	258	PRO
1	aS	123	ASN
1	bd	123	ASN
2	bz	454	SER

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Mol	Chain	Res	Type
3	bC	379	ASP
5	bE	358	VAL
7	bH	283	SER
9	bM	6	ARG
14	bT	172	ASN
14	bT	173	ALA
21	cp	264	PRO
21	cv	212	PRO
21	cv	309	THR
21	cw	263	ASN
21	cw	296	LYS
21	cE	128	PHE
21	cJ	239	LYS
21	cJ	265	ASP
24	cR	46	ASP
24	cR	47	VAL
24	cR	246	LEU
24	cS	246	LEU
24	cT	246	LEU
4	cZ	273	PHE
4	df	273	PHE
4	df	359	THR
4	dj	273	PHE
4	dl	272	PRO
4	dl	273	PHE
4	dr	30	ASN
4	dr	273	PHE
1	ad	68	THR
1	ad	69	ASP
1	ak	123	ASN
1	aq	258	PRO
1	aL	123	ASN
1	aN	123	ASN
1	bc	123	ASN
1	be	123	ASN
17	ch	14	ILE
21	cs	128	PHE
21	cw	123	ARG
21	cy	128	PHE
21	cC	128	PHE
21	cD	128	PHE
21	cF	128	PHE

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Mol	Chain	Res	Type
21	cM	264	PRO
21	cN	128	PHE
24	cS	21	PRO
24	cT	21	PRO
4	cX	272	PRO
4	cX	359	THR
23	db	9	ASN
4	dd	181	SER
4	dd	359	THR
4	df	30	ASN
4	dk	272	PRO
4	dr	22	ASN
1	aR	258	PRO
1	bb	123	ASN
4	bD	185	ILE
8	bJ	96	SER
9	bN	34	ILE
14	bX	197	ASP
21	cp	128	PHE
21	cq	255	THR
21	cr	265	ASP
21	cs	84	ALA
21	ct	267	ALA
21	cz	128	PHE
21	cD	265	ASP
21	cE	265	ASP
21	cG	265	ASP
21	cH	128	PHE
21	cK	265	ASP
21	cN	265	ASP
24	cT	46	ASP
25	cV	25	ALA
4	cX	181	SER
4	cZ	249	MET
4	cZ	272	PRO
23	db	10	PRO
4	df	181	SER
4	df	249	MET
4	dj	181	SER
4	dp	181	SER
4	dr	249	MET
1	aR	15	ASP

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Mol	Chain	Res	Type
1	aT	102	GLY
1	bd	258	PRO
1	bl	123	ASN
1	bo	257	HIS
1	bt	258	PRO
2	bx	87	THR
11	bQ	92	ALA
14	bU	160	TRP
14	bW	197	ASP
14	bY	164	ASN
16	cg	89	GLY
21	cp	309	THR
21	cD	309	THR
24	cR	21	PRO
24	cS	47	VAL
24	cT	47	VAL
4	cX	249	MET
4	dd	249	MET
4	df	193	THR
4	dk	249	MET
4	dl	46	TYR
4	dl	366	GLN
4	dp	136	ARG
4	dr	181	SER
1	as	258	PRO
1	ax	257	HIS
1	aR	257	HIS
1	bk	257	HIS
2	bA	81	GLY
4	bD	249	MET
8	bI	96	SER
9	bL	34	ILE
14	bV	196	VAL
14	bY	146	PRO
14	bY	197	ASP
4	cZ	136	ARG
4	dj	249	MET
1	ba	258	PRO
14	bT	167	GLY
1	bf	258	PRO
1	bi	258	PRO
11	bQ	88	PHE

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Mol	Chain	Res	Type
14	ce	197	ASP
4	dd	193	THR
4	dl	249	MET
5	dq	358	VAL
1	ak	257	HIS
1	aQ	257	HIS
1	bb	257	HIS
3	bC	32	GLY
14	ca	197	ASP
21	cz	294	VAL
21	cJ	294	VAL
4	cZ	181	SER
4	df	136	ARG
4	dp	193	THR
4	dp	249	MET
4	dr	193	THR
1	aP	258	PRO
1	aY	257	HIS
1	aZ	257	HIS
2	bu	120	PRO
21	cw	102	PRO
4	dd	136	ARG

5.3.2 Protein sidechains (i)

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
1	aG	357/358 (100%)	356 (100%)	1 (0%)	92 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
1	al	356/358 (99%)	356 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
1	bq	357/358 (100%)	357 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
8	bJ	122/144 (85%)	122 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
20	co	78/130 (60%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
22	di	22/1123 (2%)	22 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ab	104	ARG
1	ab	256	ASN
1	ab	419	LYS
1	ae	32	ARG
1	ah	256	ASN
1	ak	363	ARG
1	am	256	ASN
1	an	399	ASN
1	ao	62	ARG
1	as	256	ASN
1	av	76	LEU
1	aA	363	ARG
1	aD	119	LEU
1	aG	256	ASN
1	aH	325	ARG
1	aN	363	ARG
1	aV	399	ASN

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Mol	Chain	Res	Type
1	bb	363	ARG
1	bf	76	LEU
1	bk	76	LEU
1	bk	119	LEU
1	bl	63	ASN
1	bo	122	MET
1	br	419	LYS
2	bu	33	ARG
2	bu	195	GLU
2	bu	344	TRP
2	bu	374	GLU
2	bu	442	GLN
2	bv	33	ARG
2	bv	231	ARG
2	bv	362	ARG
2	bv	374	GLU
2	bv	442	GLN
2	bw	442	GLN
2	bx	231	ARG
2	bx	374	GLU
2	bx	377	PHE
2	by	79	LEU
2	bz	193	GLU
2	bz	231	ARG
2	bz	442	GLN
2	bA	160	MET
2	bA	168	ARG
2	bA	179	ARG
4	bD	200	ILE
5	bE	74	LEU
4	bF	370	LEU
9	bM	38	LYS
9	bO	53	LYS
11	bQ	183	LYS
14	ca	155	LEU
14	cc	134	PRO
14	cd	172	ASN
17	ch	128	ARG
21	cs	277	ARG
21	cx	277	ARG
21	cA	289	LYS
21	cB	289	LYS

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Mol	Chain	Res	Type
21	cC	277	ARG
21	cE	277	ARG
21	cF	70	ASN
21	cF	277	ARG
21	cG	277	ARG
21	cG	289	LYS
21	cI	277	ARG
21	cJ	156	MET
21	cK	277	ARG
21	cM	289	LYS
21	cN	101	TYR
22	cQ	27	TYR
24	cR	295	ARG
24	cS	295	ARG
4	cX	135	PHE
4	cX	293	ASP
5	cY	74	LEU
5	cY	112	ARG
4	dd	145	ARG
5	de	74	LEU
4	df	135	PHE
22	dg	15	ARG
23	dh	14	ARG
4	dj	135	PHE
4	dj	174	LYS
4	dk	62	PHE
4	dk	67	ARG
4	dk	135	PHE
4	dk	370	LEU
4	dl	370	LEU
26	do	24	ASN
5	dq	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	ac	415	ASN
1	ae	309	GLN
1	ah	63	ASN
1	aj	256	ASN
1	ak	420	ASN
1	al	14	GLN

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Mol	Chain	Res	Type
1	al	43	GLN
1	al	187	ASN
1	am	187	ASN
1	aq	187	ASN
1	ar	415	ASN
1	as	338	GLN
1	at	187	ASN
1	au	63	ASN
1	au	137	ASN
1	ay	187	ASN
1	aA	137	ASN
1	aA	187	ASN
1	aB	187	ASN
1	aC	232	GLN
1	aC	420	ASN
1	aD	187	ASN
1	aD	256	ASN
1	aE	256	ASN
1	aF	338	GLN
1	aG	187	ASN
1	aH	187	ASN
1	aI	338	GLN
1	aJ	108	HIS
1	aJ	157	GLN
1	aJ	187	ASN
1	aL	187	ASN
1	aO	338	GLN
1	aP	309	GLN
1	aQ	144	GLN
1	aR	187	ASN
1	aR	265	ASN
1	aR	267	ASN
1	aR	415	ASN
1	aT	137	ASN
1	aU	437	ASN
1	aV	321	ASN
1	aW	420	ASN
1	ba	47	ASN
1	bb	415	ASN
1	be	47	ASN
1	be	415	ASN
1	bf	144	GLN

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Mol	Chain	Res	Type
1	bh	43	GLN
1	bh	137	ASN
1	bi	256	ASN
1	bj	14	GLN
1	bj	187	ASN
1	bj	250	ASN
1	bk	187	ASN
1	bl	63	ASN
1	bm	63	ASN
1	bm	187	ASN
1	bn	309	GLN
1	bn	338	GLN
1	bn	399	ASN
1	bo	338	GLN
1	bp	187	ASN
1	bq	14	GLN
1	bs	187	ASN
1	bs	230	GLN
1	bt	137	ASN
2	bw	403	ASN
2	by	152	ASN
2	by	403	ASN
2	by	447	HIS
2	bB	483	GLN
5	bE	272	ASN
7	bH	517	ASN
8	bJ	114	GLN
13	bS	32	GLN
13	bS	166	GLN
14	bW	199	ASN
14	ca	166	GLN
14	cb	166	GLN
14	cd	166	GLN
19	cm	48	GLN
20	co	70	ASN
21	cr	122	GLN
21	cs	65	ASN
21	cs	122	GLN
21	ct	217	HIS
21	cu	69	ASN
21	cu	122	GLN
21	cv	234	HIS

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Mol	Chain	Res	Type
21	cw	122	GLN
21	cx	60	ASN
21	cB	302	GLN
21	cD	171	ASN
21	cD	302	GLN
21	cE	122	GLN
21	cL	302	GLN
21	cL	333	GLN
21	cN	122	GLN
21	cN	333	GLN
23	cP	32	ASN
22	cQ	31	ASN
24	cR	215	HIS
24	cS	349	ASN
24	cS	400	ASN
25	cU	20	ASN
25	cW	20	ASN
4	cZ	216	ASN
4	dd	45	ASN
4	df	275	ASN
22	dg	37	GLN
23	dh	9	ASN
23	dt	32	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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.

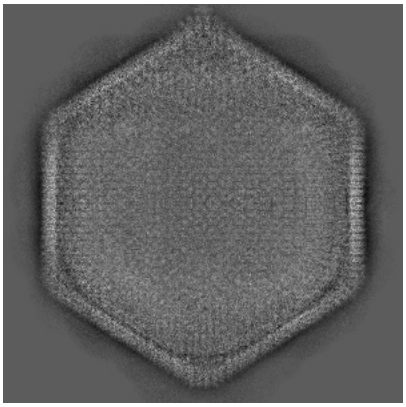
6 Map visualisation

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.

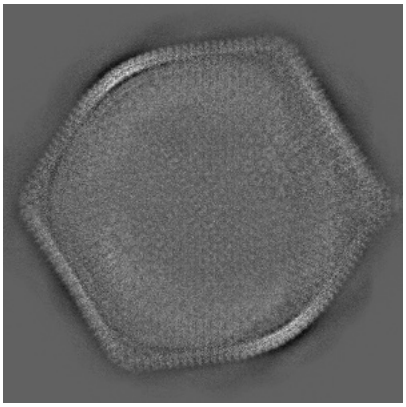
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

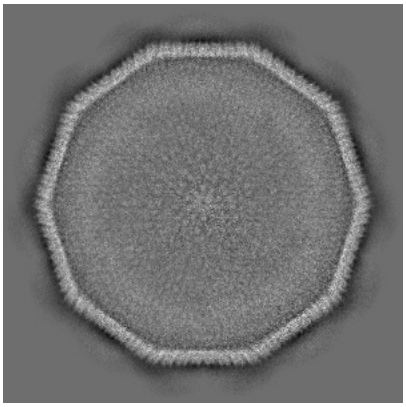
6.1.1 Primary map



X



Y

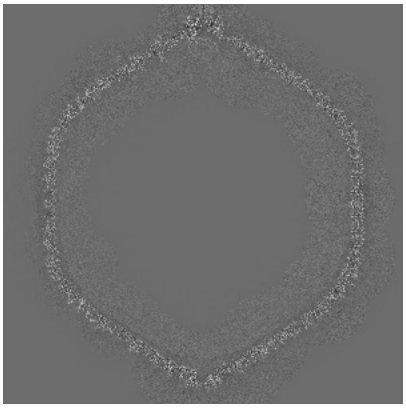


Z

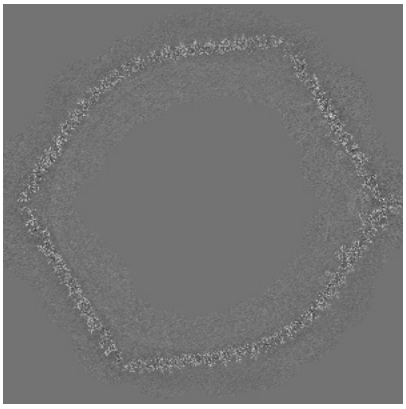
The images above show the map projected in three orthogonal directions.

6.2 Central slices

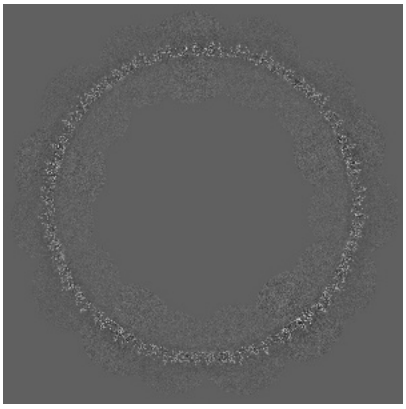
6.2.1 Primary map



X Index: 600



Y Index: 600

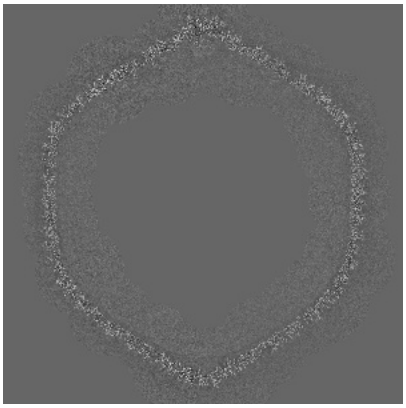


Z Index: 600

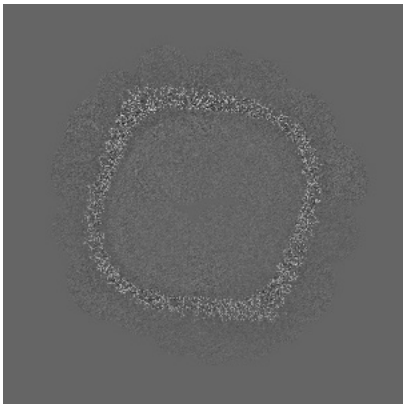
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

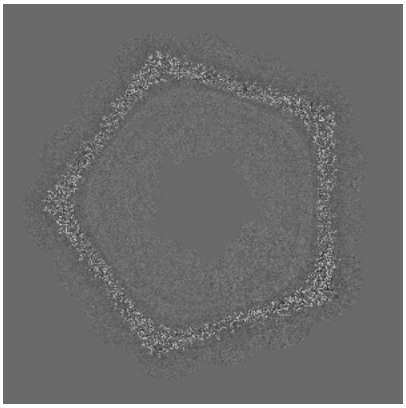
6.3.1 Primary map



X Index: 628



Y Index: 257



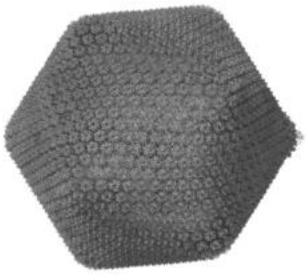
Z Index: 320

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

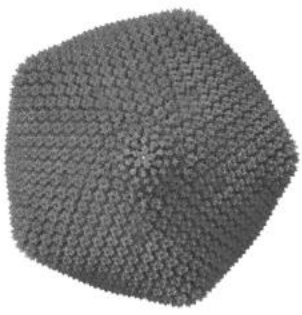
6.4 Orthogonal surface views (i)

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.

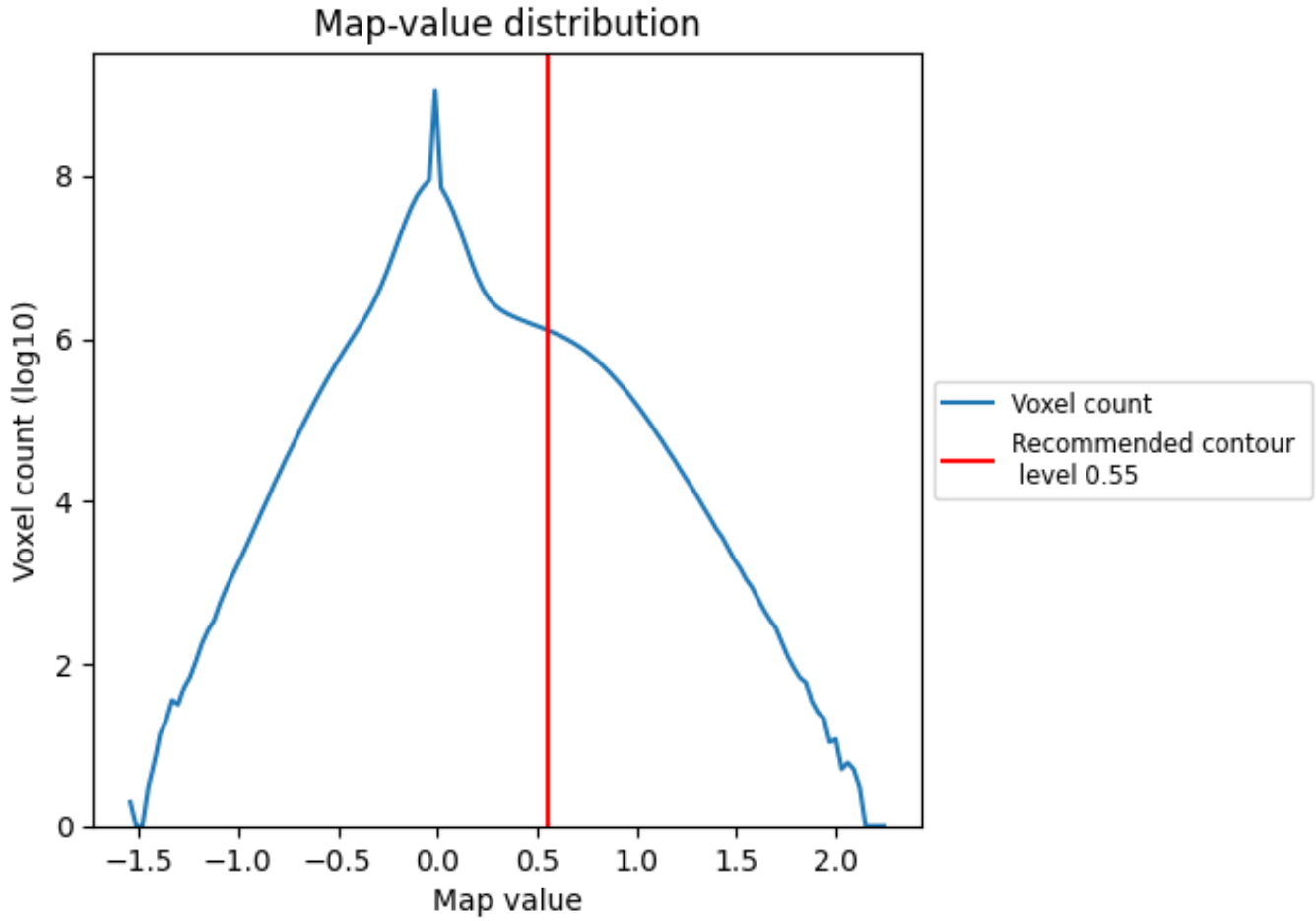
6.5 Mask visualisation (i)

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

7 Map analysis

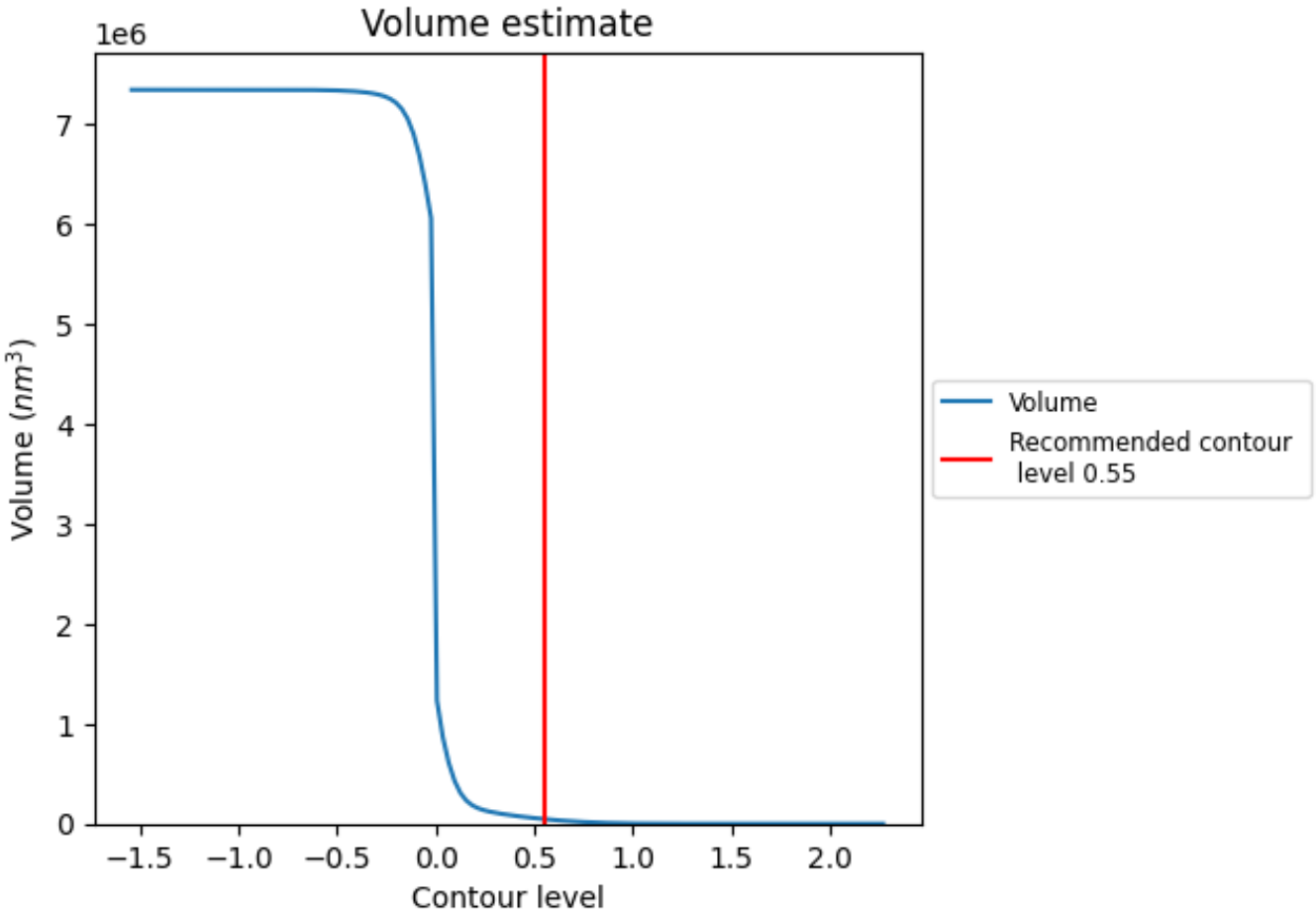
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

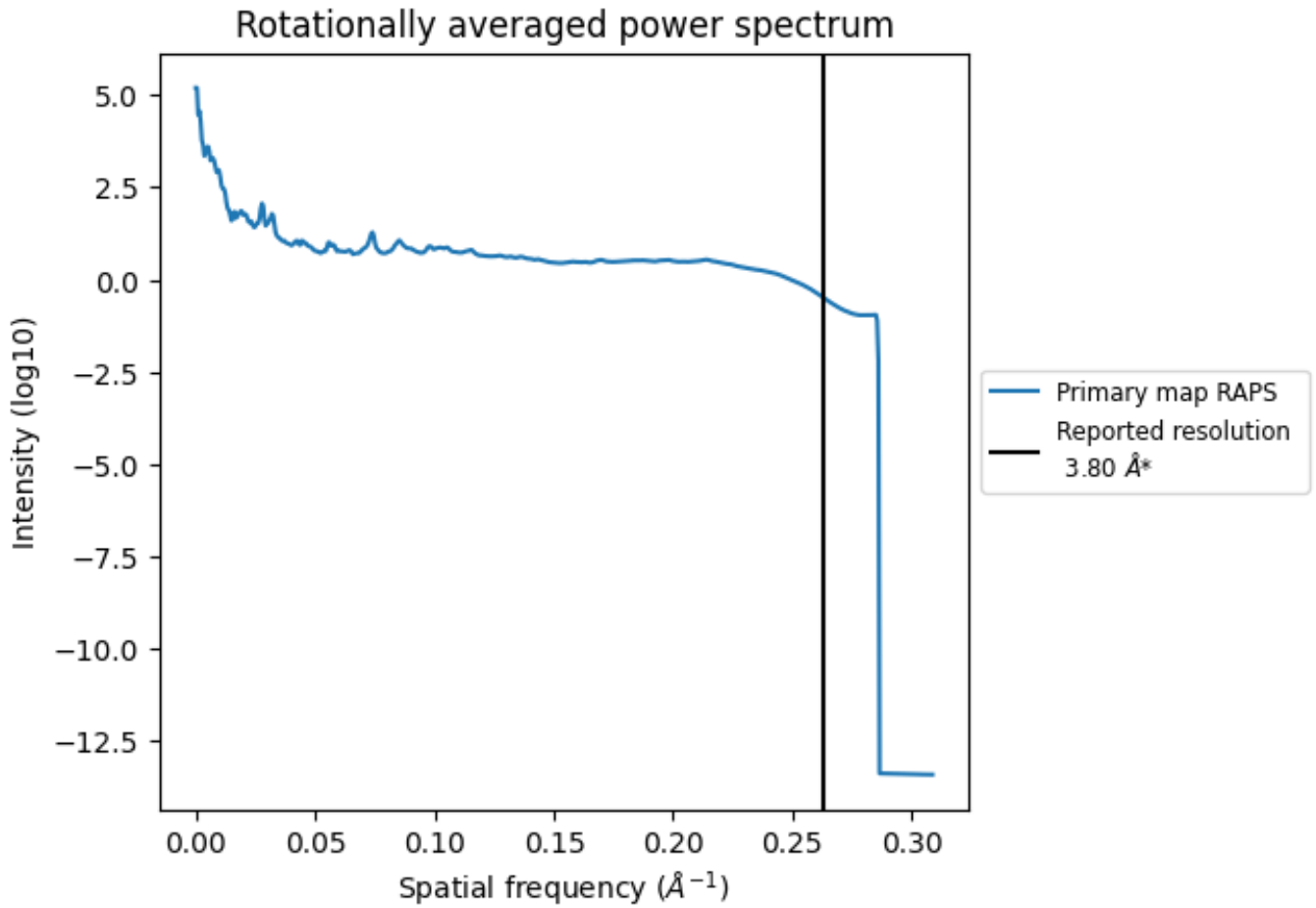
7.2 Volume estimate



The volume at the recommended contour level is 46843 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

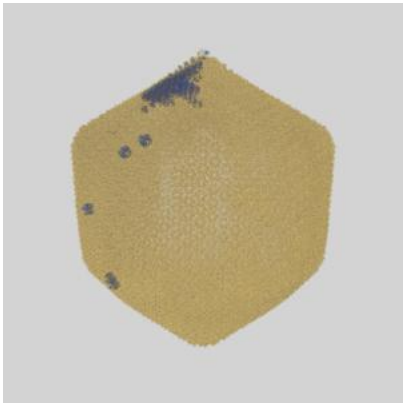
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

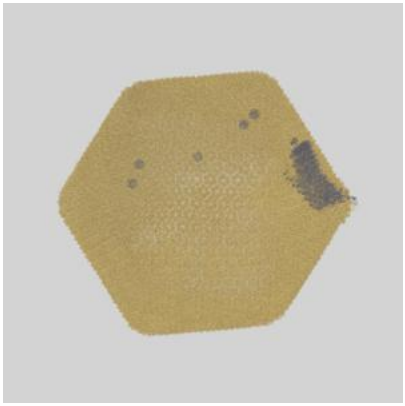
This section contains information regarding the fit between EMDB map EMD-34438 and PDB model 8H2I. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlays

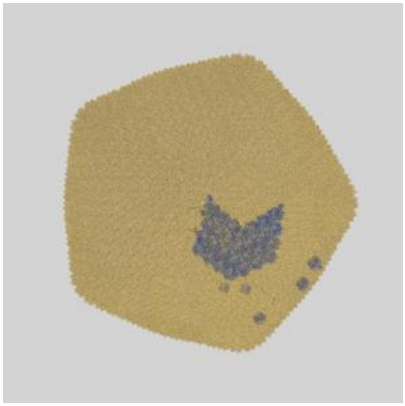
9.1.1 Map-model overlay



X

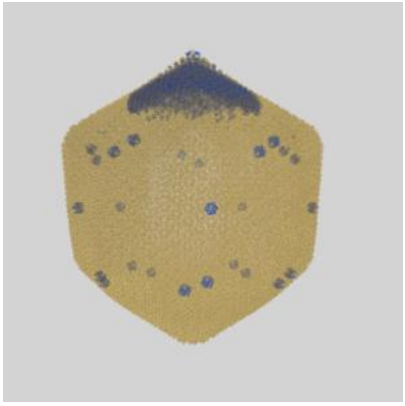


Y

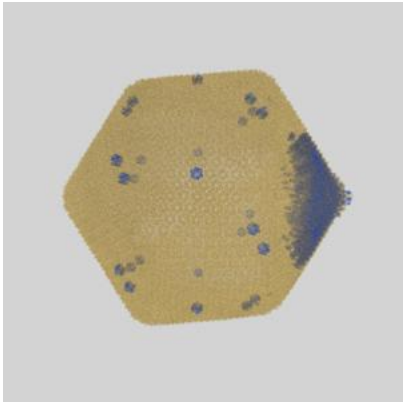


Z

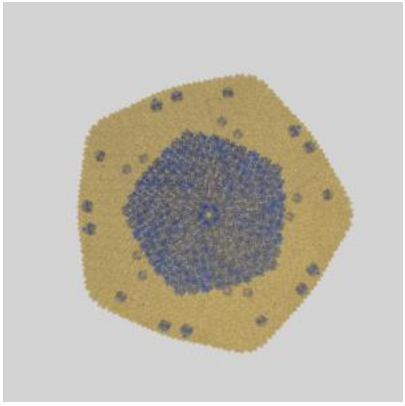
9.1.2 Map-model assembly overlay



X



Y



Z

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.

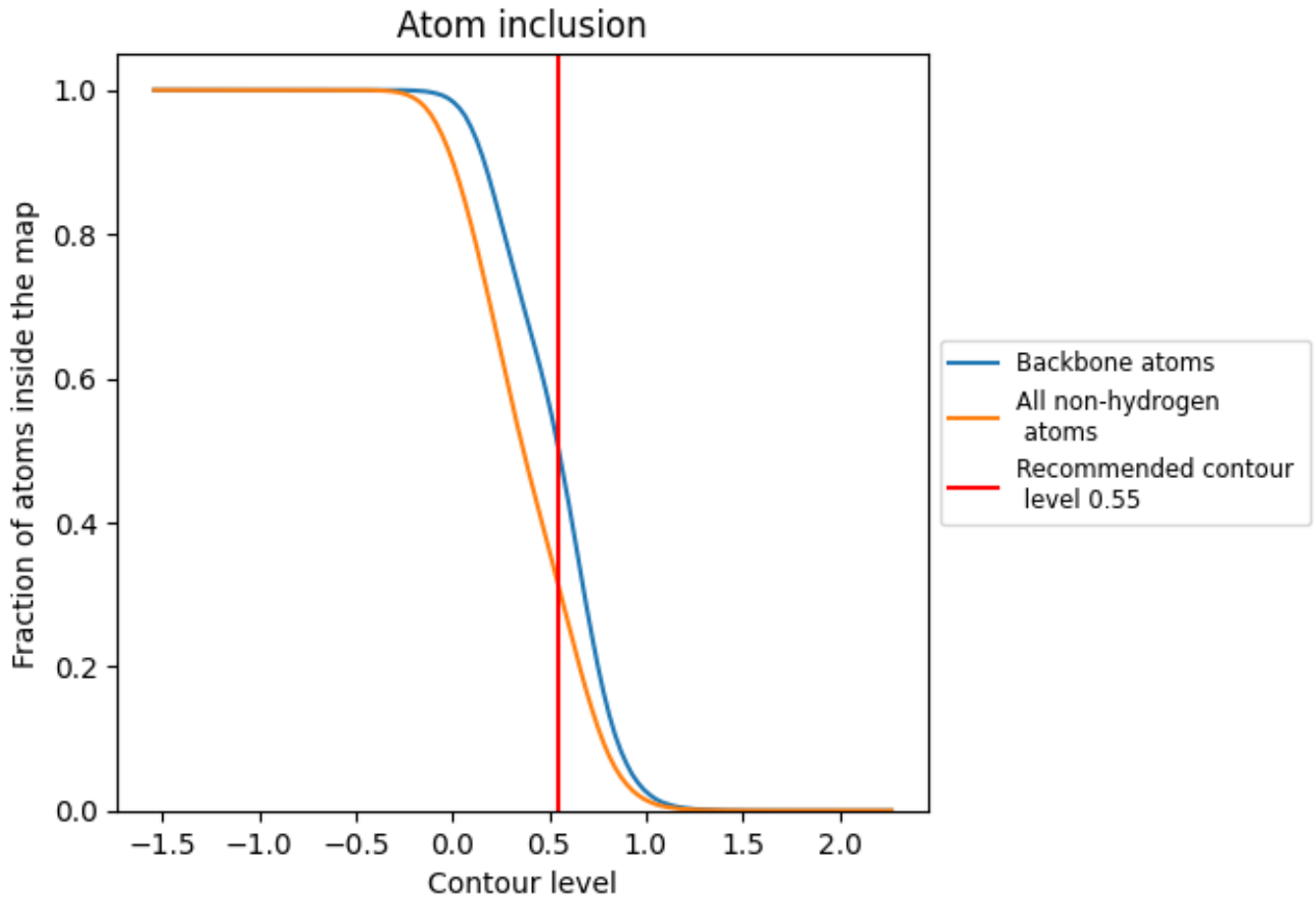
9.2 Q-score mapped to coordinate model (i)

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